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FILE COVERS 1907 - 27 Apr 2007 VOL 146 ISS 19  
FILE LAST UPDATED: 26 Apr 2007 (20070426/ED)

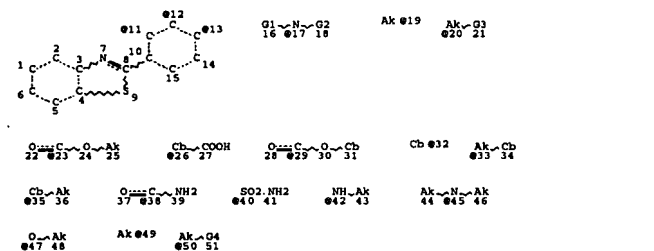
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VAR G2=49/50

VAR G3=X/NH2/42/45/CN/47/COOH

VAR G4=X/NH2/42/45/CN/47

VPA 17-11/12/13 U

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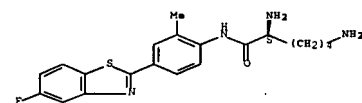
10/511,852

April 27, 2007

clonogenic survival and cell growth (growth curves but not MTS assay) endpoints. The efficacy of Phortress against colorectal cancer cells in the current study confirms that the spectrum of activity of Phortress may be wider than previously thought.

IT 328087-38-3, Phortress  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(anti-angiogenic and cytotoxic activity of Phortress against breast and colorectal cancer cells)  
RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 2005:1097667 HCAPLUS Full-text  
DOCUMENT NUMBER: 144:141573  
TITLE: Update to: The Aryl Hydrocarbon Receptor in Anticancer Drug Discovery: Friend or foe?  
AUTHOR(S): Bradshaw, T. D.; Mortimer, C. G.; Westwell, A. D.  
CORPORATE SOURCE: Centre for Biomolecular Sciences, School of Pharmacy, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Medicinal Chemistry Reviews--Online (2005), 2(2), 153-161  
CODEN: MCRRC9; ISSN: 1567-2034  
URL: <http://www.ingentaconnect.com/content/ben/mcro/2005/00000002/00000002>  
PUBLISHER: Bentham Science Publishers Ltd.  
DOCUMENT TYPE: Journal; General Review; (online computer file)  
LANGUAGE: English

AB A review. Major advances in our understanding of the mechanistic features and regulation of Aryl hydrocarbon Receptor (Ahr) mediated signal transduction have been made in recent years. This review updates our previously published article "The Aryl Hydrocarbon Receptor in Anticancer Drug Discovery: Friend or Foe?", focussing on the most recent developments in the field. Discussion of receptor regulation and crosstalk, structural studies on the ligand binding domain, the search for endogenous ligands, and therapeutic possibilities in the cancer field associated with Ahr ligands, feature prominently here.

IT 328087-38-3, Phortress  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

CONNECT IS E2 RC AT 33  
CONNECT IS E1 RC AT 34  
CONNECT IS E2 RC AT 35  
CONNECT IS E1 RC AT 36  
CONNECT IS E1 RC AT 43  
CONNECT IS E1 RC AT 44  
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CONNECT IS E1 RC AT 48  
CONNECT IS E1 RC AT 49  
DEFAULT MLLEVEL IS ATOM  
GGCAT IS UNS AT 26  
GGCAT IS UNS AT 31  
GGCAT IS UNS AT 32  
GGCAT IS UNS AT 34  
GGCAT IS UNS AT 35  
DEFAULT ECLLEVEL IS LIMITED  
ECOUNT IS M5 C AT 49  
ECOUNT IS M5 C AT 50

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 51

STEREO ATTRIBUTES: NONE

L9 33 SEA FILE=REGISTRY SSS FUL L7  
L10 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

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L10 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 2006:1210169 HCAPLUS Full-text  
DOCUMENT NUMBER: 146:155514  
TITLE: In vitro cytotoxicity of Phortress against colorectal cancer  
AUTHOR(S): Mukherjee, Abhik; Graham Martin, Stewart  
CORPORATE SOURCE: Department of Oncology, City Hospital, University of Nottingham, Nottingham, NG5 1PB, UK  
SOURCE: International Journal of Oncology (2006), 29(5), 1287-1294  
CODEN: IJONES; ISSN: 1019-6439  
PUBLISHER: International Journal of Oncology  
DOCUMENT TYPE: Journal  
LANGUAGE: English

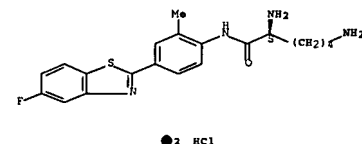
AB Phortress is a novel benzothiazole compound with activity concentrated in certain breast, ovarian and renal cancer cell lines. Its anti-angiogenic effects are unknown. In this study, the in vitro anti-angiogenic effects of Phortress were screened for and results compared with two control drugs, paclitaxel and fumagillin. In vitro anti-angiogenic activity was examined by MTS assays, growth curves and clonogenic survival assays on human umbilical vein endothelial cells (HUVEC). In addition and as a comparator, effects were examined on MRCV fibroblasts and also the MCF7 breast cancer cell line, shown to be sensitive on the MCF7 panel and 3 colorectal cancer cell lines (HT29, SW480 and SW620) that were reportedly insensitive. Effects on endothelial tube differentiation were assessed by the Matrigel assay. Phortress had no effect on HUVEC and MRCV cell proliferation and survival. Unlike paclitaxel and fumagillin, Phortress did not inhibit endothelial tube differentiation. Phortress therefore exhibits no in vitro anti-angiogenic activity. As expected, Phortress was cytotoxic to MCF7 breast cancer cells, but unexpectedly, Phortress was also potent against colorectal cancer cells in

10/511,852

April 27, 2007

(aryl hydrocarbon receptor agonist, 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole, active component of prodrug Phortress binding induced CYP1A1 which converted it to cytotoxic intermediate thus can be used in patient with cancer)  
RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 2005:6103 HCAPLUS Full-text  
DOCUMENT NUMBER: 142:385200  
TITLE: In vitro, in vivo, and in silico analyses of the antitumor activity of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazoles  
AUTHOR(S): Leong, Chee Onn; Suggitt, Marie; Swaine, David J.; Bibby, Michael C.; Stevens, Malcolm F. G.; Bradshaw, Tracey D.  
CORPORATE SOURCE: Centre for Biomolecular Sciences, School of Pharmacy, University of Nottingham, Nottingham, UK  
SOURCE: Molecular Cancer Therapeutics (2004), 3(12), 1565-1575  
CODEN: MCTOCP; ISSN: 1535-7163  
PUBLISHER: American Association for Cancer Research  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Phortress is a novel, potent, and selective exptl. antitumor agent. Its mechanism of action involves induction of CYP1A1-catalyzed biotransformation of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole (5F 203) to generate electrophilic species, which covalently bind to DNA, exacting lethal damage to sensitive tumor cells, in vitro and in vivo. Herein, we investigate the effects of DNA adduct formation on cellular DNA integrity and progression through cell cycle and examine whether a relevant pharmacodynamic end point may be exploited to probe the clin. mechanism of action of Phortress and predict tumor response. Single cell gel electrophoresis (SCGE) was applied to quantify DNA damage and cell cycle analyses conducted upon 5F 203 treatment of benzothiazole-sensitive MCF-7 and inherently resistant MDA-MB-435 breast carcinoma cells. Following treatment of xenograft-bearing mice and mice possessing hollow fiber implants containing MCF-7 or MDA-MB-435 cells with Phortress (20 mg/kg, i.p., 24 h), tumor cells and xenografts were recovered for analyses by SCGE. Dose- and time-dependent DNA single and double strand breaks occurred exclusively in sensitive cells following treatment with 5F 203

in vitro (10 nmol/L-10  $\mu$ mol/L; 24-72 h). In vivo, Phortress-sensitive and Phortress-resistant tumor cells were distinct; moreover, DNA damage in xenografts, following treatment of mice with Phortress, could be determined. Interrogation of the mechanism of action of 5F 203 in silico by self-organizing map-based cluster analyses revealed modulation of phosphatases and kinases associated with cell cycle regulation, corroborating observations of selective cell cycle perturbation by 5F 203 in sensitive cells. By conducting SCGE, tumor sensitivity to Phortress, an agent currently undergoing clinical evaluation, may be determined.

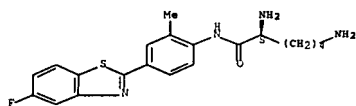
## IT 328087-38-3, Phortress

RL: DNA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (in vitro, in vivo, and in silico analyses of antitumor activity of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazoles)

RN 328087-38-3 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

## Absolute stereochemistry.



●2 HCl

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 13

HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:757951 HCAPLUS Full-text

DOCUMENT NUMBER: 142:348246

TITLE:

The Experimental Antitumor Agents Phortress and Doxorubicin are Quasiactive Against Human-Derived Breast Carcinoma Xenograft Models  
Fichtner, Iduna; Monks, Anne; Hesse, Curtis; Stevens, Malcolm F. G.; Bradshaw, Tracey D.

CORPORATE SOURCE: Max-Delbrueck Center for Molecular Medicine,

Experimental Pharmacology, Berlin, Germany

SOURCE: Breast Cancer Research and Treatment (2004), 87(1),

97-107

CODEN: BCTRD6; ISSN: 0167-6806

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Phortress (the dihydrochloride salt of the lysylamide prodrug of 2-(4-amino-3-methylphenyl)-5-fluoro-benzothiazole (5F 203)) is an exptl. antitumor agent with potent and selective activity against human-derived carcinomas of breast, ovarian and renal origin. The mechanism of action of Phortress is distinct from all classes of chemotherapeutic agents currently in the clinic, and involves metabolic activation by cytochrome P 450 (CYP) 1A1 to electrophilic

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species, which generate DNA adducts in sensitive tumors only. In the present study, the antitumor efficacy of Phortress has been compared with that of doxorubicin (Dox) in nine human-derived mammary carcinoma xenograft models, cultivated s.c. in the flanks of nude mice. In addition, cyp1a1 mRNA expression was measured in tumors of control and treated animals. Phortress compared favorably with Dox: significant activity, independent of estrogen receptor (ER) status, was established in 7/9 xenografts; in one xenograft model, Phortress elicited superior antitumor activity; no model demonstrated complete resistance to Phortress. In accordance with this observation, all xenografts available for examination (8) displayed clear induction of cyp1a1 expression upon treatment of mice with Phortress whereas Dox failed to induce cyp1a1 expression in all models. Prolonged viability of tumor fragments, recovered for treatment ex vivo could not be sustained; thus correlations between tumor cells' response to Phortress and cyp1a1 or cyp1b1 inducibility following 5F 203 treatment could not be determined with confidence.

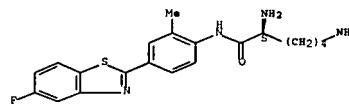
IT 328087-38-3, NSC 710305

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Phortress; exptl. antitumor agents Phortress and doxorubicin are equiactive against human-derived breast carcinoma xenograft models)

RN 328087-38-3 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

## Absolute stereochemistry.



●2 HCl

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 13

HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:836808 HCAPLUS Full-text

DOCUMENT NUMBER: 139:327931

TITLE:

Aminophenyl-benzothiazole compounds as UV filters in cosmetics  
Wagner, Barbara; Ehlig, Thomas; Mongiat, Sebastien; Eichin, Kai

PATENT ASSIGNER(S): Ciba Specialty Chemicals Holding Inc., Switz.

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

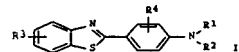
PATENT NO. KIND DATE APPLICATION NO. DATE

6

WO 2003086341	A2	20031023	WO 2003-EP3870	20030414
WO 2003086341	A3	20040401		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CO, CI, CM, GA, GN, GG, ML, MR, NE, NG, SD, TG				
AU 2003229665	A1	20031027	AU 2003-229665	20030414
EP 1494641	A2	20050112	EP 2003-722472	20030414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009308	A	20050215	BR 2003-9308	20030414
CN 1466507	A	20050727	CN 2003-804538	20030414
US 2005175554	A1	20050811	US 2003-511852	20030414
JP 2005529869	T	20051006	JP 2003-383965	20030414
IN 2004CN02585	A	20070302	IN 2004-CN2585	20041117
PRIORITY APPL. INFO.: EP 2002-405111 A 20020417				
CH 2002-2135 A 20021216				
WO 2003-EP3870 W 20030414				

OTHER SOURCE(S): MARPAT 139:327931

OI



AB The preparation and use, as a UV filter, of a compound of formula I (R1, R2 = H, unsubstituted or halo-, amino-, mono- or di-C1-5-alkylamino-, cyano- or C1-5-alkoxy-substituted C1-22-alkyl, C5-10-cycloalkyl, carboxy-C1-22-alkyl, carboxy-C6-10-aryl, C6-10-aryl, C6-10-aryl-C1-5-alkyl, carbamoyl, sulfonyl; R1, R2, N forming 5- to 7-membered heterocyclic radical; R3 = H, C1-22-alkyl; R4 = H, OH, C1-22-alkoxy) is described. The compounds of formula I in micronized form are suitable as UV absorbers in cosmetic preps. and for protecting hair and skin from UV radiation.

IT 614717-93-OP 614717-94-1P 614717-96-3P

614717-97-4P 614717-98-6P 614718-00-2P

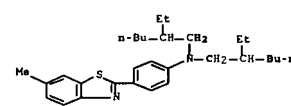
614718-02-4P 614718-04-6P 614718-05-7P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PRP (Preparation); USES (Uses) (preparation and cosmetic use of aminophenyl benzothiazole compds. as UV filters)

RN 614717-93-0 HCAPLUS

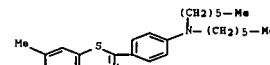
CN Benzenamine, N,N-bis(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)

7



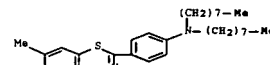
RN 614717-94-1 HCAPLUS

CN Benzenamine, N,N-dihexyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



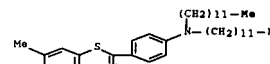
RN 614717-96-3 HCAPLUS

CN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-N,N-dioctyl- (9CI) (CA INDEX NAME)



RN 614717-97-4 HCAPLUS

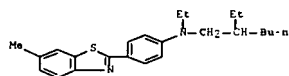
CN Benzenamine, N,N-didodecyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



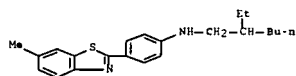
RN 614717-99-6 HCAPLUS

CN Benzenamine, N-ethyl-N-(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)

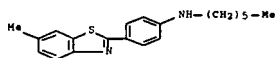
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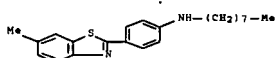
RN 614718-00-2 HCAPLUS  
CN Benzenamine, N-(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



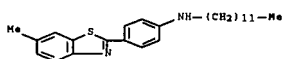
RN 614718-02-4 HCAPLUS  
CN Benzenamine, N-hexyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 614718-04-6 HCAPLUS  
CN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-N-octyl- (9CI) (CA INDEX NAME)

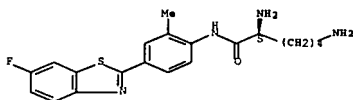


RN 614718-05-7 HCAPLUS  
CN Benzenamine, N-dodecyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 328087-39-4 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

L10 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:87659 HCAPLUS Full-text  
DOCUMENT NUMBER: 139:316727  
TITLE: Antitumour 2-(4-aminophenyl)benzothiazoles generate DNA adducts in sensitive tumour cells in vitro and in vivo

AUTHOR(S): Leong, C.-O.; Gaskell, M.; Martin, E. A.; Heydon, R. T.; Farmer, P. B.; Bibby, M. C.; Cooper, P. A.; Double, J. A.; Bradshaw, T. D.; Stevens, M. F. G.

CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: British Journal of Cancer (2003), 88(3), 470-477  
CODEN: BJCAAI; ISSN: 0007-0920

PUBLISHER: Nature Publishing Group  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB 2-(4-Aminophenyl)benzothiazoles represent a potent and highly selective class of antitumor agent. In vitro, sensitive carcinoma cells deplete 2-(4-aminophenyl)benzothiazoles from nutrient media; cytochrome P 450 1A1 activity, critical for execution of antitumor activity, and protein expression are powerfully induced. 2-(4-Amino-3-methylphenyl)benzothiazole-derived covalent binding to cytochrome P 450 1A1 is reduced by glutathione, suggesting 1A1-dependent production of a reactive electrophilic species. In vitro, 2-(4-aminophenyl)benzothiazole-generated DNA adducts form in sensitive tumor cells

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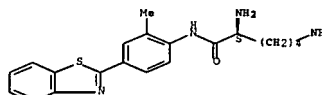
L10 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:241156 HCAPLUS Full-text  
DOCUMENT NUMBER: 140:35389  
TITLE: Preclinical evaluation of amino acid prodrugs of novel antitumor 2-(4-amino-3-methylphenyl)benzothiazoles. [Erratum to document cited in CA137:72775]  
AUTHOR(S): Bradshaw, Tracey D.; Bibby, Michael C.; Double, John A.; Fichtner, Iduna; Cooper, Patricia A.; Alley, Michael C.; Donohue, Susan; Stinson, Sherman P.; Tomaszewski, Joseph E.; Sausville, Edward A.; Stevens, Malcolm F. G.  
CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Molecular Cancer Therapeutics (2003), 2(2), 207  
CODEN: MCTOCF; ISSN: 1535-7163  
PUBLISHER: American Association for Cancer Research  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB In Figure 3, panels B and C were transposed; the corrected figure is given.  
IT 328087-34-9 328087-38-3 328087-39-4

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preclin. evaluation of amino acid prodrugs of antitumor 2-(4-amino-3-methylphenyl)benzothiazoles (Erratum))

RN 328087-34-9 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

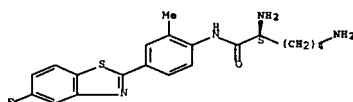


●2 HCl

RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

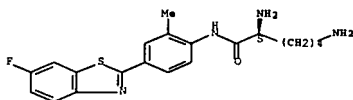
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●2 HCl

RN 328087-39-4 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

L10 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:87659 HCAPLUS Full-text  
DOCUMENT NUMBER: 139:316727  
TITLE: Antitumour 2-(4-aminophenyl)benzothiazoles generate DNA adducts in sensitive tumour cells in vitro and in vivo

AUTHOR(S): Leong, C.-O.; Gaskell, M.; Martin, E. A.; Heydon, R. T.; Farmer, P. B.; Bibby, M. C.; Cooper, P. A.; Double, J. A.; Bradshaw, T. D.; Stevens, M. F. G.

CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: British Journal of Cancer (2003), 88(3), 470-477  
CODEN: BJCAAI; ISSN: 0007-0920

PUBLISHER: Nature Publishing Group  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB 2-(4-Aminophenyl)benzothiazoles represent a potent and highly selective class of antitumor agent. In vitro, sensitive carcinoma cells deplete 2-(4-aminophenyl)benzothiazoles from nutrient media; cytochrome P 450 1A1 activity, critical for execution of antitumor activity, and protein expression are powerfully induced. 2-(4-Amino-3-methylphenyl)benzothiazole-derived covalent binding to cytochrome P 450 1A1 is reduced by glutathione, suggesting 1A1-dependent production of a reactive electrophilic species. In vitro, 2-(4-aminophenyl)benzothiazole-generated DNA adducts form in sensitive tumor cells

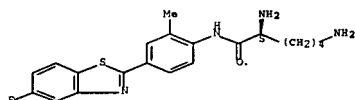
11

only. At concns. >100 nM, adducts were detected in DNA of MCF-7 cells treated with 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole (SF 203). SF 203 (1 μM) led to the formation of one major and a number of minor adducts. However, treatment of cells with 10 μM SF 203 resulted in the emergence of a new dominant adduct. Adducts accumulated steadily within DNA of MCF-7 cells exposed to 1 μM SF 203 between 2 and 24 h. Concns. of the lysylamide prodrug of SF 203 (Phortress) 2100 nM generated adducts in the DNA of sensitive MCF-7 and IGROV-1 ovarian cells. At 1 μM, one major Phortress-derived DNA adduct was detected in these two sensitive phenotypes; 10 μM Phortress led to the emergence of an addnl. major adduct detected in the DNA of MCF-7 cells. Inherently resistant MDA-MB-435 breast carcinoma cells incurred no DNA damage upon exposure to Phortress (510 μM, 24 h). In vivo, DNA adducts accumulated within sensitive ovarian IGROV-1 and breast MCF-7 xenografts 24 h after treatment of mice with Phortress (20 mg kg<sup>-1</sup>). Moreover, Phortress-derived DNA adduct generation distinguished sensitive MCF-7 tumors from inherently resistant MDA-MB-435 xenografts implanted in opposite flanks of the same mouse.

IT 328087-38-3, NSC 710305  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(antitumor 2-(4-aminophenyl)benzothiazoles generate DNA adducts in sensitive tumor cells in vitro and in vivo)

RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2002:440574 HCAPLUS Full-text  
DOCUMENT NUMBER: 138:49377

TITLE: In vitro evaluation of amino acid prodrugs of novel antitumor 2-(4-amino-3-methylphenyl)benzothiazoles  
AUTHOR(S): Bradshaw, T. D.; Chua, M.-S.; Browne, H. L.; Trapani, V.; Sausville, E. A.; Stevens, M. F. G.

CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: British Journal of Cancer (2002), 86(8), 1348-1354  
CODEN: BJCAAI; ISSN: 0007-0920

PUBLISHER: Nature Publishing Group

12

DOCUMENT TYPE:  
LANGUAGE:Journal  
English

AB Novel 2-(4-aminophenyl)benzothiazoles possess highly selective, potent antitumor properties in vitro and in vivo. They induce and are biotransformed by cytochrome P 450 (CYP) 1A1 to putative active as well as inactive metabolites. Metabolic inactivation of the mol. has been thwarted by isosteric replacement of hydrogen with fluorine atoms at positions around the benzothiazole nucleus. The lipophilicity of these compds. presents limitations for drug formulation and bioavailability. To overcome this problem, water soluble prodrugs have been synthesized by conjugation of alanyl- and lysyl-amide hydrochloride salts to the exocyclic primary amine function of 2-(4-aminophenyl)benzothiazoles. The prodrugs retain selectivity with significant in vitro growth inhibitory potency against the same sensitive cell lines as their parent amine, but are inactive against cell lines inherently resistant to 2-(4-aminophenyl)benzothiazoles. Alanyl and lysyl prodrugs rapidly and quant. revert to their parent amine in sensitive and insensitive cell lines in vitro. Liberated parent compds. are sequestered and metabolized by sensitive cells only; similarly, CYP1A1 activity and protein expression are selectively induced in sensitive carcinoma cells. Amino acid prodrugs meet the criteria of aqueous solubility, chemical stability and quant. reversion to parent mol., and thus are suitable for in vivo preclin. evaluation.

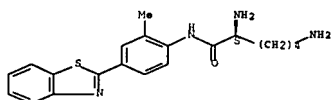
IT 328087-34-9 328087-38-3 328087-39-4  
328087-50-9

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(in vitro evaluation of amino acid prodrugs of novel antitumor amino methylphenyl benzothiazoles)

RN 328087-34-9 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

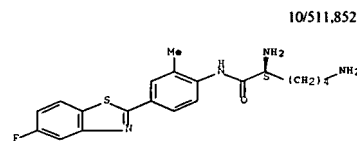


●2 HCl

RN 328087-38-3 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

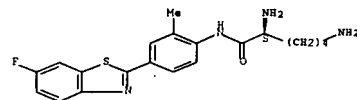


●2 HCl

RN 328087-39-4 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(6-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

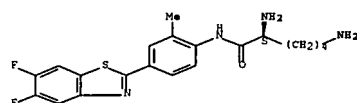


●2 HCl

RN 328087-50-9 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5,6-difluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

REFERENCE COUNT:

17

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2007 ACS ON STN

13

14

ACCESSION NUMBER: 2002:210849 HCAPLUS Full-text  
DOCUMENT NUMBER: 137:72775  
TITLE: Preclinical evaluation of amino acid prodrugs of novel antitumor 2-(4-amino-3-methylphenyl)benzothiazoles  
AUTHOR(S): Bradshaw, Tracey D.; Bibby, Michael C.; Double, John A.; Fichtner, Iduna; Cooper, Patricia A.; Alley, Michael C.; Donohue, Susan; Stinson, Sherman P.; Tomaszewski, Joseph E.; Sausville, Edward A.; Stevens, Malcolm P. G.  
CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Molecular Cancer Therapeutics (2002), 1(4), 239-246  
CODEN: MCTOCF; ISSN: 1535-7163  
PUBLISHER: American Association for Cancer Research  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Novel 2-(4-aminophenyl)benzothiazoles possess highly selective, potent antitumor properties in vitro and in vivo. Elucidation of the mechanism of action of this structurally simple class of compds. has occurred in parallel with selection of a candidate clin. agent. Antitumor benzothiazoles induce and are biotransformed by cytochrome P 450 1A1 to putative active, as well as inactive metabolites. Metabolic inactivation of the mol. has been thwarted by isosteric replacement of hydrogen with fluorine atoms at positions around the benzothiazole nucleus. Amino acid conjugation to the exocyclic primary amine function of 2-(4-aminophenyl)benzothiazoles has been used to overcome limitations posed by drug lipophilicity. Water soluble, chemical stable prodrugs rapidly and quant. revert to their parent amine in mice, rats, and dogs in vivo. Plasma concns. of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole regenerated from the lysylamide prodrug (1), sufficient to elicit cytotoxic activity against ZR-75-1 and T47D human mammary carcinoma cell lines persist > 6 h. The growth of breast (MCF-7) and ovarian (IGROV-1) xenograft tumors is significantly retarded by 1. Manageable toxic side effects are reported from pre-clin. efficacious doses of 1. Cytochrome P 450 1A1 protein expression, selectively induced in sensitive carcinoma cells, was detected in MCF-7 and IGROV-1 tumors 24 h after treatment of mice with 1 (20 mg/kg). The lysyl amide prodrug of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole is potentially suitable for clin. evaluation.

IT 328087-34-9 328087-38-3 328087-39-4

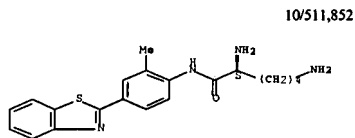
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preclin. evaluation of amino acid prodrugs of antitumor 2-(4-amino-3-methylphenyl)benzothiazoles)

RN 328087-34-9 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

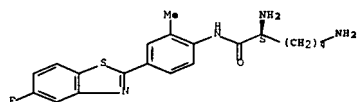


●2 HCl

RN 328087-38-3 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

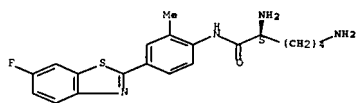


●2 HCl

RN 328087-39-4 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(6-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

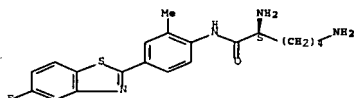
L10 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2007 ACS ON STN

15

16

ACCESSION NUMBER: 2001:918063 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:184083  
 TITLE: Antitumor Benzothiazoles. 16. Synthesis and Pharmaceutical Properties of Antitumor 2-(4-Aminophenyl)benzothiazole Amino Acid Prodrugs  
 AUTHOR(S): Hutchinson, Ian; Jennings, Sharon A.; Vishnuvajjala, B. Rao; Westwell, Andrew D.; Stevens, Malcolm F. G.  
 CORPORATE SOURCE: Cancer Research Laboratories School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
 SOURCE: Journal of Medicinal Chemistry (2002), 45(3), 744-747  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:184083  
 AB A series of water-soluble L-lysyl- and L-alanyl-amide prodrugs of the lipophilic antitumor 2-(4-aminophenyl)benzothiazole has been synthesized to address formulation and bioavailability issues related to the desired parenteral administration of the chosen clin. candidate. The prodrugs exhibit the required pharmaceutical properties of good water solubility (in weak acid) and stability at ambient temperature and degradation to free base in vivo. The lysyl-amide of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole (NSC 710305) has been selected for phase 1 clin. evaluation.  
 IT 328087-38-3P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (synthesis of antitumor (aminophenyl)benzothiazole amino acid prodrugs)  
 RN 328087-38-3 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

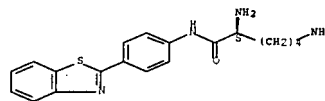


●2 HCl

IT 328087-33-8P 328087-34-9P 328087-35-0P  
 328087-39-4P 328087-50-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of antitumor (aminophenyl)benzothiazole amino acid prodrugs)  
 RN 328087-33-8 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)phenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

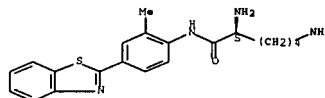
17



●2 HCl

RN 328087-34-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

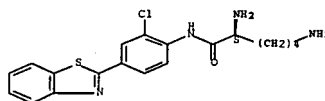
Absolute stereochemistry.



●2 HCl

RN 328087-35-0 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-chlorophenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

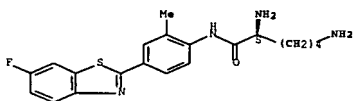


●2 HCl

RN 328087-39-4 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(6-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

18

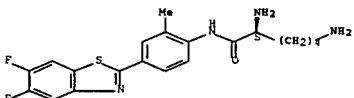
Absolute stereochemistry.



●2 HCl

RN 328087-50-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5,6-difluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

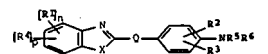
L10 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:152462 HCAPLUS Full-text  
 DOCUMENT NUMBER: 134:193429  
 TITLE: Preparation of substituted 2-phenylbenzothiazoles as antitumor agents  
 INVENTOR(S): Stevens, Malcolm Francis Graham; Poole, Tracey Dawn; Westwell, Andrew David; Hutchinson, Ian Paul; Chua, Mei-sze  
 PATENT ASSIGNER(S): Cancer Research Campaign Technology Limited, UK  
 SOURCE: PCT Int. Appl., 58 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001014354	A1	20010301	WO 2000-GB3210	20000821
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

19

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW  
 RM: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CO, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TO  
 CA 2382406 A1 20010301 CA 2000-2382406 20000821  
 EP 1204650 A1 20020515 EP 2000-954726 20000821  
 EP 1204650 B1 20060419  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL  
 JP 2003507462 T 20030225 JP 2001-518442 20000821  
 AU 783360 B2 20051020 AU 2000-67085 20000821  
 AT 232686 T 20060515 AT 2000-954726 20000821  
 PT 1204650 T 20060831 PT 2000-954726 20000821  
 ES 2263483 T3 20061216 ES 2000-954726 20000821  
 US 6858633 B1 20050222 US 2002-69018 20020729  
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 GB 1998-19673 A 19990820  
 WO 2000-GB3210 W 20000821

OTHER SOURCE(S): MARPAT 134:193429  
 GI

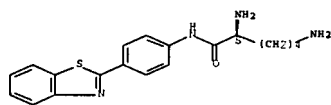


AB The title compds. [I; X = S, O; Q = a direct bond, CH2, CH; R1 = halo, CF3, SmMe3; R2 = H, NO2, N3, etc.; R3 = H, halo, alkyl, etc.; R4 = alkyl, haloalkyl, OH, etc.; R5, R6 = H, amino acid residue, alkyl, etc.; p = 0-2; n = 0-3] which exhibit selective antiproliferative activity in respect of mammalian tumor cells, were prepared e.g., a 4-step synthesis of I [X = S; Q = a direct bond; R1 = 4-F; R2 = 3-Me; R3-R6 = H] (starting with 3-methyl-4-nitrobenzoyl chloride and 2-fluorobenzoaniline) which showed IC50 of <0.1 nM and of 0.13 nM in MCF-7 and MDA468 cell lines, resp., was given. At least in preferred compds. I the benzene ring of the benzothiazole nucleus has a halogen substituent, preferably fluorine, and the 2-Ph group has a 4'-amino substituent which may be conjugated with an amino acid to provide a water soluble amino acid amide prodrug or its salt.

IT 328087-33-8P 328087-34-9P 328087-35-0P  
 328087-38-3P 328087-39-4P 328087-50-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of substituted 2-phenylbenzothiazoles as antitumor agents)  
 RN 328087-33-8 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)phenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

20

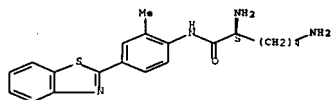


● 2 HCl

RN 328087-34-9 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

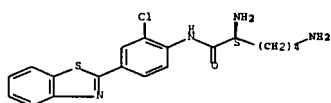


● 2 HCl

RN 328087-35-0 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-chlorophenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



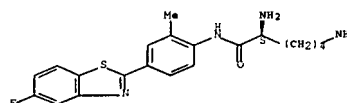
● 2 HCl

RN 328087-36-3 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

21

Absolute stereochemistry.

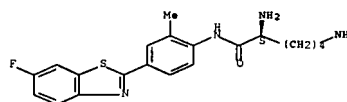


● 2 HCl

RN 328087-39-4 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

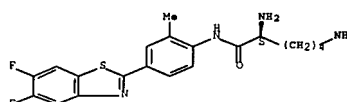


● 2 HCl

RN 328087-50-9 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5,6-difluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

22

L10 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:465965 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 65:65965  
 ORIGINAL REFERENCE NO.: 65:12316g-h, 12317a-b  
 TITLE: 4,4'-Dibenzamido-6,6'-alkylsulfonylstilbene-3,3'-disulfonic acids  
 PATENT ASSIGNER(S): J. R. Geigy A.-G.  
 SOURCE: 11 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1031750		19660602	GB 1964-51648	19641218
FR 1426394			FR	
PRIORITY APPLN. INFO.:			CH	19631220

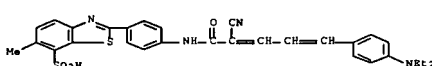
GI For diagram(s), see printed CA Issue.

AB Comps. of the general formula I are fluorescent brightening agents with improved chlorine fastness. Reduction of 4,2-Cl(Me)C<sub>6</sub>H<sub>3</sub>SO<sub>2</sub>Cl with Na<sub>2</sub>SO<sub>3</sub> gives 4,2-Cl(Me)C<sub>6</sub>H<sub>3</sub>SO<sub>2</sub>H, methylated with Me<sub>2</sub>SO<sub>4</sub> to give 4,2-Cl(Me)C<sub>6</sub>H<sub>3</sub>SO<sub>2</sub>Me (II), m. 70°. Nitration of II in H<sub>2</sub>SO<sub>4</sub> gives 4,2,5-Cl(Me)C<sub>6</sub>H<sub>3</sub>SO<sub>2</sub>Me, m. 137°, which, treated with Na<sub>2</sub>SO<sub>3</sub>, gives 5,2,4-Me(O<sub>2</sub>N)(MeSO<sub>2</sub>)C<sub>6</sub>H<sub>2</sub>SO<sub>3</sub>H, oxidized with aqueous NaOCl to [2,4,5-MeSO<sub>2</sub>(O<sub>2</sub>N)(HO<sub>3</sub>S)C<sub>6</sub>H<sub>2</sub>CH:]<sub>2</sub> which is reduced to [2,4,5-MeSO<sub>2</sub>(H<sub>2</sub>N)(HO<sub>3</sub>S)C<sub>6</sub>H<sub>2</sub>CH:]<sub>2</sub> (III). A suspension of 40 vols. III in 400 vols. anhydrous pyridine treated with a solution of 40 parts 4,2-Me(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>COCl (IV) in 50 parts anhydrous PhMe, refluxed for 2 hrs. at 100-10°, treated with a solution of 40 parts IV in 50 parts PhMe, heated 2 hrs. at 100-10°, cooled, filtered, washed with C<sub>6</sub>H<sub>6</sub>, dried, stirred into 1200 parts 5% aqueous Na<sub>2</sub>CO<sub>3</sub> at 70-80°, cooled, filtered, and washed with 2.5% aqueous NaCl gives I (X = OEt, Y = Me, Z = H). Similarly, other I are prepared (X, Y, and Z given): MeO, MeO, H; MeO, Me, Me; H, AcNH, H; H, EtO<sub>2</sub>CNH, H; HO, Me, H; HOCH<sub>2</sub>CH<sub>2</sub>O, Me, H; H, O<sub>2</sub>N, H; H, H<sub>2</sub>.

IT 10189-99-SP, 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, sodium salt  
 10210-90-SP, 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, sodium salt  
 RL: PREP (Preparation)

RN 10189-99-9 HCAPLUS

CN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, monosodium salt (8CI) (CA INDEX NAME)



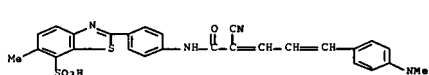
● Na

RN 10210-90-9 HCAPLUS

CN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, monosodium salt (8CI) (CA INDEX NAME)

23

2,4-pentadienamido]phenyl]-7-methyl-, monosodium salt (8CI) (CA INDEX NAME)



● Na

L10 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:465964 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 65:65964  
 ORIGINAL REFERENCE NO.: 65:12316d-g  
 TITLE: Substantive methine dyes  
 INVENTOR(S): Cohen, Werner V.  
 PATENT ASSIGNER(S): E. I. du Pont de Nemours & Co.  
 SOURCE: 5 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3257394		19660621	US 1962-218146	19620820
PRIORITY APPLN. INFO.:			US	19620820

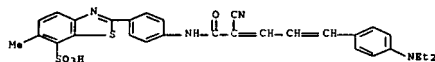
GI For diagram(s), see printed CA Issue.

AB The title compts., aromatic sulfonic acids containing O groups as substituents, are greenish yellow dyes for paper which turn red on acidification. They are prepared by condensing 4-R(R')NCH<sub>2</sub>CHO with cyanoacetylides. Thus, a mixture of [4,2-NCH<sub>2</sub>CO<sub>2</sub>NH(NaO<sub>3</sub>S)C<sub>6</sub>H<sub>3</sub>CH:]<sub>2</sub> 5.5, 4-Me<sub>2</sub>NCH<sub>2</sub>CHO 3.0, EtOH 16.0, and piperidine 0.15 part is heated at refluxing temperature for 3 hrs., cooled, filtered, washed with EtOH, and dried to give [4,2-Q(NaO<sub>3</sub>S)C<sub>6</sub>H<sub>3</sub>CH:]<sub>2</sub> (I, R = R' = Me, n = 0), bright green-yellow on paper pulp, green fluorescence under uv light, red on alum-treated paper, λ<sub>2</sub>20max. 438 mμ λ<sub>2</sub>MeOHmax. 418 mμ. Similarly, other I (n = 0) are prepared (R, R', λ<sub>2</sub>20max. and λ<sub>2</sub>MeOHmax. in μ given): 6, Me, Me, 0.436, 417; 6, Et, Et, 0.443, 425; 6, Me, Et, 0.439, 422; 6, Et, CH<sub>2</sub>CH<sub>2</sub>OH, 0.436, 424; 6, Me, CH<sub>2</sub>CH<sub>2</sub>OH, 0.440, 418. Similarly, x.1.3-Q(HO)C<sub>10</sub>H<sub>5</sub>SO<sub>3</sub>Na are prepared (x, R, R', n, λ<sub>2</sub>20max. and λ<sub>2</sub>MeOHmax. in μ given): 6, Me, Me, 0.436, 417; 6, Et, Et, 0.443, 425; 6, Me, Et, 0.439, 422; 6, Et, CH<sub>2</sub>CH<sub>2</sub>OH, 0.436, 424; 6, Me, CH<sub>2</sub>CH<sub>2</sub>OH, 0.440, 418. Similarly, x.1.3-Q(HO)C<sub>10</sub>H<sub>5</sub>SO<sub>3</sub>Na are prepared (x, R, R', n, λ<sub>2</sub>20max. and λ<sub>2</sub>MeOHmax. in μ given): 6, Me, Me, 0.447, 423; 6, Et, Et, 0.452, 430; 6, Me, Et, 0.450, 428; 6, Et, CH<sub>2</sub>CH<sub>2</sub>OH, 0.448, 427; 6, Et, CH<sub>2</sub>Ph, 0.438, 420; 6, Me, I, 503.466 (scarlet on paper); 6, Et, 1.490, 487. Also prepared is 1,3,6-HO(NaO<sub>3</sub>S)C<sub>10</sub>H<sub>5</sub>NHCO<sub>2</sub>(CN):CHC<sub>6</sub>H<sub>3</sub>(NMe<sub>2</sub>)Me-4,2, λ<sub>2</sub>20max. 454 mμ λ<sub>2</sub>MeOHmax. 436 mμ. The dyes are soluble in HCONMe<sub>2</sub>, but only slightly soluble in H<sub>2</sub>O.

IT 10189-99-SP, 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, sodium salt

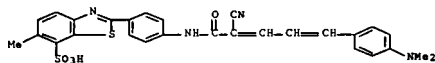
24

10210-90-9P, 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, sodium salt  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 10189-99-8 HCAPLUS  
 CN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, monosodium salt (8CI) (CA INDEX NAME)



● Na

RN 10210-90-9 HCAPLUS  
 CN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-7-methyl-, monosodium salt (8CI) (CA INDEX NAME)



● Na

=> fil marpat

FILE 'MARPAT' ENTERED AT 13:05:02 ON 27 APR 2007  
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FILE CONTENT: 1961-PRESENT VOL 146 ISS 16 (20070420/ED)

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MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES  
 (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2007055070 08 MAR 2007  
 DE 102005041140 01 MAR 2007  
 EP 1760076 07 MAR 2007  
 JP 2007055923 08 MAR 2007  
 WO 2007030409 15 MAR 2007  
 GB 2429455 28 FEB 2007  
 FR 2890072 02 MAR 2007

25

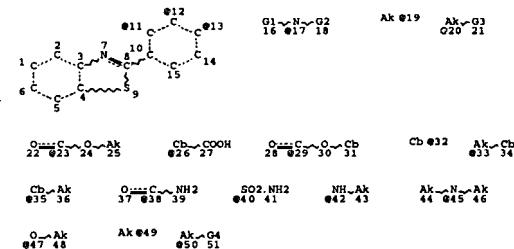
RU 2294322 27 FEB 2007  
 CA 2556850 24 FEB 2007

Expanded G-group definition display now available.

=> d que 123

L7

STR



VAR G1-H/19/20/23/26/29/32/33/35/38/40

VAR G2-49/50

VAR G3-X/NH2/42/45/CN/47/COOH

VAR G4-X/NH2/42/45/CN/47

VPA 17-11/12/13 U

MODE ATTRIBUTES:

CONNECT IS E1 RC AT 19

CONNECT IS E1 RC AT 25

CONNECT IS E2 RC AT 26

CONNECT IS E1 RC AT 31

CONNECT IS E1 RC AT 32

CONNECT IS E2 RC AT 33

CONNECT IS E1 RC AT 34

CONNECT IS E2 RC AT 35

CONNECT IS E1 RC AT 36

CONNECT IS E1 RC AT 43

CONNECT IS E1 RC AT 44

CONNECT IS E1 RC AT 46

CONNECT IS E1 RC AT 48

CONNECT IS E1 RC AT 49

DEFAULT MLEVEL IS ATOM

OGCAT IS UNS AT 26

OGCAT IS UNS AT 31

OGCAT IS UNS AT 32

OGCAT IS UNS AT 34

OGCAT IS UNS AT 35

DEFAULT ELEVEL IS LIMITED

BCOUNT IS MS C AT 49

BCOUNT IS MS C AT 50

GRAPH ATTRIBUTES:

26

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 51

STEREO ATTRIBUTES: NONE

L9 SEA FILE-REGISTRY SSS PUL L7  
 L10 13 SEA FILE-HCAPLUS ABB-ON PLU-ON L9  
 L22 36 SEA FILE-MARPAT SSS PUL L7  
 L33 34 SEA FILE-MARPAT ABB-ON PLU-ON L22 NOT L10

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L23 ANSWER 1 OF 34 MARPAT COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER:

TITLE: Process for fluorination of anilides

INVENTOR(S): Storey, Anthony Ramon; Jones, Clare Louise; Bouvet, Denis Raymond Christophe; Laebistes, Nicolas; Fairway, Steven Michael; Williams, Lorenzo; Gibson, Alexander Mark; Nairne, Robert James; Karimi, Farhad; Langstrom, Bengt

PATENT ASSIGNER(S): GE Healthcare Limited, UK; GE Healthcare A/S

SOURCE: PCT Int. Appl., 45pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGES: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

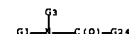
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007020400	A1	20070222	WO 2006-093009	20060811
W: AS, AO, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, DE, DK, DM, DZ, EC, EE, ES, FI, FR, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TO, BW, GH, GM, KE, LS, MW, ME, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPL. INFO.: GB 2005-16564 20050812				

OTHER SOURCE(S):

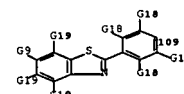
AB This invention relates to a process for preparing fluorinated anilines with general formula of F-A-NH-R [wherein A = Ph with optional 1-4 substituents; R = alkyl, alkenyl, or alkynyl], which comprises reacting fluoride, suitably [18F]fluoride, with the corresponding anilides, followed by removal of protecting groups to give the title compounds. For example, precursor I (preparation given) was fluoridized using (Kryptofix 2.2.2)potassium fluoride-18F (preparation given), followed by hydrolysis in methanol in the presence of concentrated hydrochloric acid to give II. The 18F-labeled compds. are useful as in vivo imaging agents for positron emission tomog. (PET) (no data).

MSTR 2

27



G1 = 109



G3 = Me

G4 = F

G24 = alkyl <containing 1-10 C>

(opt. substd. by 1 or more G4)

Patent location: claim 1

Note: or protected derivatives

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RS FORMAT

L23 ANSWER 2 OF 34 MARPAT COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 146:184430 MARPAT Full-text

TITLE: 2-Arylbenzothiazole analogs as kinase inhibitors and their preparation, pharmaceutical compositions and use in the treatment of kinase-mediated diseases  
 INVENTOR(S): Ehlert, Jan; Herz, Thomas; Krause, Rolf; Kubbutat, Michael; Lang, Martin; Saeb, Wael; Schaechele, Christoph; Tasler, Stefan; Totzke, Frank; Zirrgebel, Ute

PATENT ASSIGNER(S): ASC AG, Germany

SOURCE: U.S. Pat. Appl. Publ., 47pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGES: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

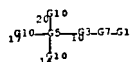
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2007021446	A1	20070125	US 2006-434658	20060516
PRIORITY APPL. INFO.: US 2005-699656P 20050715				

AB The invention relates to compds. of the general formula I and salts, produgs, and stereoisomers thereof. Compds. of formula I wherein Y is S, O, NH and deriva., SO and SO2; A is (un)substituted 5- to 6-membered (hetero)aromatic ring; R1 is (un)substituted quinolinyl, (un)substituted quinoxalinyl, (un)substituted isoquinolinyl, (un)substituted pyridinyl, (un)substituted pyridinyl, etc.; R5 - R7 are independently H, CHO, acyl, CO2H and deriva., SOH and deriva., SO2H and deriva., SO3H and deriva., NO2, CN, CF3, etc.; and their pharmaceutically acceptable salts, produgs and stereoisomers thereof, are claimed. Example compound II was prepared amination of 2-halo-3,5-

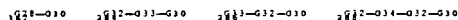
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dimethylpyrimidine with 4-(benzothiazol-2-yl)phenylamine. All the invention compds. were evaluated for their kinase inhibitory activity (data given).

## MSTR 1



G2 = 362 / 284 / 286 / 288



G3 = p-C6H4 (opt. substd. by 1 or more G4)  
G5 = 3-10 9-17 8-20 7-14



G7 = 260



G28 = carbon chain <containing 1-6 C,  
0 or more double bonds, 0 or more triple bonds>  
(opt. substd.)

G29 = NH2  
G30 = 293



Patent location: claim 1  
Note: substitution is restricted  
Note: additional ring and oxo formation also claimed

L23 ANSWER 3 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 146:184428 MARPAT Full-text  
TITLE: Preparation of 2-heteroarylaminothiophenylbenzothiazoles  
as anticancer drugs.

29

G3 = p-C6H4 (opt. substd. by 1 or more G4)  
G5 = 3-10 9-17 8-20 7-14



G7 = 260



G28 = carbon chain <containing 1-6 C,  
0 or more double bonds, 0 or more triple bonds>  
(opt. substd.)

G29 = NH2  
G30 = 293



Patent location: claim 1  
Note: substitution is restricted  
Note: additional ring and oxo formation also claimed

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 146:154716 MARPAT Full-text  
TITLE: Preparation of transition metal thiosemicarbazone derivative complexes for medical imaging and therapy  
INVENTOR(S): Heslop, Jonathan Robin; Peach, Josephine Mary;  
Heslop, Julia May; Donnelly, Paul Stephen  
PATENT ASSIGNEE(S): Isis Innovation Limited, UK  
SOURCE: PCT Int. Appl., 132pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007003944	A2	20070111	WO 2006-02488	20060705
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,				

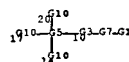
31

INVENTOR(S): Ehler, Jan; Herz, Thomas; Krauss, Rolf; Kubbutat, Michael; Lang, Martin; Saeb, Wael; Schaechtele, Christoph; Taeler, Stefan; Totzke, Frank; Zirrgiebel, Ute  
PATENT ASSIGNEE(S): 4SC AG, Germany  
SOURCE: Eur. Pat. Appl., 74pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

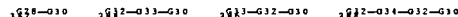
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1746096	A1	20070124	EP 2005-15432	20050715
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WO 2007009524	A1	20070125	WO 2006-EP4620	20060516
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VM, YU, ZA, ZM, ZW				
RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NS, SN, TD, TO, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: EP 2005-15432 20050715  
AB Title compds. [I; Y = S, O, NR2, SO, SO2; A = divalent (substituted) aryl, heteroaryl; R1 = specified isoquinolinyl, quinolinyl, pyrimidinyl, pyridyl, etc.; R2 = H, alkyl, cycloalkyl, hydroxyalkyl, haloalkyl, aminoalkyl, cyano, COR11, etc.; R3-R7 = H, COR11, COR11, SO2R11, NO2, cyano, CF3, OCF3, alkyl, cycloalkyl, alkoxy, amino, (substituted) aryl, heteroaryl, etc.; R11 = H, alkyl, cycloalkyl, amino, (substituted) aryl, heteroaryl, etc.; with proviso(s)], were prepared. Thus, 4-benzothiazol-2-ylphenylamine and 4-chloropicolinic acid were heated together at 160° for 3 h to give 84 (4-benzothiazol-2-ylphenyl)pyridin-4-ylamine. Several I inhibited cellular receptor tyrosine kinase and/or cellular Aurora-B kinase with IC50 <10 μM.

## MSTR 1



G2 = 362 / 284 / 286 / 288

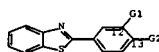


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MM, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW  
RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NS, SN, TD, TO, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2005-13812 20050705  
AB Metal thiosemicarbazone derivative complexes I (M is a transition metal and A1, A2, X, X', Y, L1', R1' and R2' are defined) are prepared and are useful in medical imaging and therapy. The complexes are hypoxic selective. The preparation and fluorescence of a number of mononuclear examples compound, e.g., zinc(II) complex II, as well as dinuclear complexes of bis(thiosemicarbazone) derivs. are included.

## MSTR 2



G2 = 21



G4 = alkyl <containing 1-10 C> (substd. by 1 or more G5)  
G5 = F  
Patent location: claim 27

L23 ANSWER 5 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 144:488685 MARPAT Full-text  
TITLE: Heteroaryl compounds, particularly N-heteroaryl hydrazones, their preparation, and their therapeutic use as IL-12 production inhibitors  
INVENTOR(S): Sun, Lijun; Zhang, Shijie; Koya, Keisuke; Chimmannamada, Dinesh; Li, Hao; James, David; Kostik, Elena  
PATENT ASSIGNEE(S): Synta Pharmaceuticals Corp., USA  
SOURCE: PCT Int. Appl., 172 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006053109	A1	20060518	WO 2005-USA0706	20051110
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,				

32



CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MM, MX, MZ, NA, NG, NI, NO, NZ, OM, PA, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

AB The invention is related to the preparation of heteroaryl compounds I (Q, U, V = independently N, CH and deriv.; Z = H, NH<sub>2</sub> and deriv.; OH and deriv.; (un)substituted cycloalkyl, etc.; X = O, S, SO, CO, N=N, NHC=O, etc.; R = R'-L'-R''; R' = (un)substituted cycloalkyl, cyclyl, aryl, etc.; L' = O, S, NH and deriv.; absent, etc.; R'' = H, OH and deriv.; halo, CN, alkyl, aryl, etc.; R1 = (CR2R4)n-O-R3; Y = CO, O, S, NH and deriv.; absent, etc.; R3 = H, (un)substituted alk(en)ynyl, heteroaryl, OSO<sub>2</sub>H, CHO, etc.; R2, R4 for each occurrence = independently (un)substituted alkyl, alkylcarbonyl, OH and deriv.; NO, halo, CN, etc.; G = NH-C(NH)-NH, NH-CO-NH, NH-CS-NH, heteroarylene, absent, etc.; n = 0-7), and pharmaceutically acceptable salts, solvates, clathrates, hydrates, prodrugs, and polymorphs thereof. The invention is also related to methods of modulating IL-12 production and processes mediated by IL-12. E.g., a 4-step synthesis from 2,4,6-trichloropyrimidine and diethylamine was given for hydrazone 11. 1 inhibited IL-12 production in human PBMC cells and THP-1 cell line in an in vitro assay. Thus, I are useful for treating or preventing disorders related with excessive bone loss, methods for inhibiting osteoclast formation, and methods for treating or preventing a disorder associated with excessive bone resorption.

US 2006122156 A1 20060608

US 2005-271704 20051110

US 2004-627001P 20041110

PRIORITY APPLN. INFO.:  
AB The invention is related to the preparation of heteroaryl compounds I (Q, U, V = independently N, CH and deriv.; Z = H, NH<sub>2</sub> and deriv.; OH and deriv.; (un)substituted cycloalkyl, etc.; X = O, S, SO, CO, N=N, NHC=O, etc.; R = R'-L'-R''; R' = (un)substituted cycloalkyl, cyclyl, aryl, etc.; L' = O, S, NH and deriv.; absent, etc.; R'' = H, OH and deriv.; halo, CN, alkyl, aryl, etc.; R1 = (CR2R4)n-O-R3; Y = CO, O, S, NH and deriv.; absent, etc.; R3 = H, (un)substituted alk(en)ynyl, heteroaryl, OSO<sub>2</sub>H, CHO, etc.; R2, R4 for each occurrence = independently (un)substituted alkyl, alkylcarbonyl, OH and deriv.; NO, halo, CN, etc.; G = NH-C(NH)-NH, NH-CO-NH, NH-CS-NH, heteroarylene, absent, etc.; n = 0-7), and pharmaceutically acceptable salts, solvates, clathrates, hydrates, prodrugs, and polymorphs thereof. The invention is also related to methods of modulating IL-12 production and processes mediated by IL-12. E.g., a 4-step synthesis from 2,4,6-trichloropyrimidine and diethylamine was given for hydrazone 11. 1 inhibited IL-12 production in human PBMC cells and THP-1 cell line in an in vitro assay. Thus, I are useful for treating or preventing disorders related with excessive bone loss, methods for inhibiting osteoclast formation, and methods for treating or preventing a disorder associated with excessive bone resorption.

MBTR 1B



G1 = 7

G2

G3 = 12 / 1058

G4

G6 = G25

33

G7 = G25  
G25 = benzothiazolyl  
G52 = 1082-2 1083-1059



G53 = alkyl (containing 1-12 C)  
Patent location: claim 1  
Note: substitution is restricted  
Note: additional substitution also claimed  
Note: or pharmaceutically acceptable salts, solvates, clathrates, hydrates, or polymorphs

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

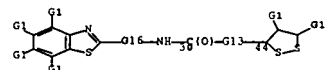
L23 ANSWER 6 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 144:219303 MARPAT Full-text  
TITLE: Amyloid-binding, metal-chelating agents  
INVENTOR(S): Huang, Kudong; Krensky, Jonathan L.; Catchings, Perry L.  
PATENT ASSIGNEE(S): The General Hospital Corporation, USA; Prime Organics, Inc.  
SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 762,965.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006035946	A1	20060216	US 2005-96919	20050401
US 2004204344	A1	20041014	US 2004-762965	20040122
PRIORITY APPLN. INFO.:			US 2003-441719P	20030122
			US 2004-762965	20040122

AB The present invention relates to the diagnosis, prevention, and treatment of pathophysiol. conditions associated with amyloid accumulation. Bifunctional therapeutic mole. and contrast imaging agents exhibiting a high affinity for amyloid deposits, and pharmaceutical compns. thereof are described. The invention also provides methods of using these bifunctional mole., contrast imaging agents, and pharmaceutical compns. for detecting the presence of amyloid deposits using imaging techniques; and for preventing or treating amyloid-related conditions, such as, for example, Alzheimer's disease.

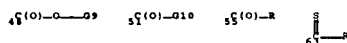
MBTR 2

34



G18

G1 = I / CN / alkyl (containing 1-6 C) / CP3 / CO<sub>2</sub>H / 48 / 51 / CH<sub>2</sub>CH<sub>2</sub>OH / 55 / 63 / CH<sub>2</sub>Ph



G13 = carbon chain (containing 4 or more C) (opt. substd. by (1-4) G1)

G16 = phenylene (opt. substd.)

Patent location: claim 5  
Note: S- or N-oxides or quaternary amines  
Note: substitution is restricted  
Note: and complex chelates with G18 metals

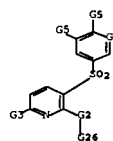
L23 ANSWER 7 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 141:366132 MARPAT Full-text  
TITLE: Preparation of pyridinyl derivatives as corticotropin releasing factor receptor 1 antagonists for the treatment of depression  
INVENTOR(S): Hartz, Richard A.; Arvanitis, Argyrios G.  
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
SOURCE: U.S. Pat. Appl. Publ., 39 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004209917	A1	20041021	US 2004-799784	20040312
US 7030145	B2	20060418		

PRIORITY APPLN. INFO.:  
AB The title compds. I (B = CH, N; D = CH<sub>2</sub>, NH; R1 = H, CH, alkyl, cycloalkyl, etc.; R2 = H, halo, CN, etc.; R3 = H, halo, CN, OH, etc.; Ar = Ph, indanyl, pyridyl, etc.) which are antagonists of the corticotropin releasing factor receptor type 1 (CRF-R1) useful for the treatment of depression, anxiety, affective disorders, feeding disorders, post-traumatic stress disorder, headache, drug addiction, inflammatory disorders, drug or alc. withdrawal symptoms and other conditions, were prepared E.g., a multi-step synthesis of 11, starting from 6-methyl-2-pyridone, was given. The compds. I demonstrated a Ki value of less than about 10,000 nM for the inhibition of CRF in the CRF-R1 receptor binding assay. The pharmaceutical composition comprising the compound I is claimed.

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MBTR 1



G1 = CH  
G5 = 30 / 41 / benzothiazolyl

G18-G19

G11 = 28

G16-G17

G16 = alkylene (containing 1 or more C) (opt. substd.)  
G17 = OMe  
G19 = 32

G18-G19

G20 = NH  
Patent location: claim 1  
Note: or pharmaceutically acceptable salts or solvates

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 141:106491 MARPAT Full-text  
TITLE: Preparation of new uracils having a herbicidal activity  
INVENTOR(S): Meazza, Giovanni; Paravidino, Piero; Betterini, Franco; Fornara, Luca  
PATENT ASSIGNEE(S): Isagro Ricerca S.r.l., Italy  
SOURCE: PCT Int. Appl., 122 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English

36

FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056785	A2	20040708	WO 2003-EP14469	20031215
WO 2004056785	A3	20040923		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RM: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TO

CA 2506826 A1 20040708 CA 2003-2506826 20031215

AU 2003294894 A1 20040714 AU 2003-294894 20031215

EP 1585737 A2 20051019 EP 2003-785868 20031215

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

BR 2003017086 A 20051025 BR 2003-17086 20031215

CN 1729177 A 20060201 CN 2003-80106868 20031215

JP 2006516126 T 20060622 JP 2004-561343 20031215

US 2006025591 A1 20060202 US 2005-536485 20050824

IN 2005DN02216 A 20061229 IN 2005-DN02216 20050825

PRIORITY APPL. INFO.: IT 2005-M12759 20021223

WO 2003-EP14469 20031215

OTHER SOURCE(S): CASREACT 141:106491

AB The title compds. I [X1 = H, halo; X2 = halo; X4 = haloalkyl; R = H, alkyl, haloalkyl; G = O, S; X3 = Q(CR1R2)nZ, Q12, Q2, Y(OC)CR6:CR5CR3R4Z; Z = O, S; R1-R4 = H, alkyl, haloalkyl; R5 = OR7; R6 = H, alkyl; R7 = alkyl, haloalkyl; Y = OR8, SR9, NR10R11; R8, R9 = H, alkyl, cycloalkyl, etc.; R10, R11 = H, alkyl, haloalkyl, etc.; n = 1-3; Q = pyrrolyl, imidazolyl, pyrazolyl, etc.; Q1 = thiazolyl, tetrazolyl, oxadiazolyl, etc.; Q2 = tetrazolyl, thiazolyl, isothiazolyl, etc.], useful as herbicides, especially for the pre-emergence and/or post-emergence control of monocotyledonous or dicotyledonous weeds, were prepared. Thus, reacting Et 3-amino-4,4,4-trifluoro-2-butenate with Me (2E)-4-(2-chloro-4-fluoro-5-isocyanatophenoxy)-3-methoxybut-2-enoate (preparation given) in the presence of NaH in DMF afforded Me (2E)-4-[2-chloro-4-fluoro-5-(1,2,3,6-tetrahydro-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl)phenoxy]-3-methoxybut-2-enoate. The herbicidal activity of the compds. I was evaluated (data given for representative compds. I). Herbicidal compds. comprising the compound I along with other herbicides (list of herbicides given), fungicides, insecticides, acaricides, fertilizers, etc., are claimed.

MSTR 2

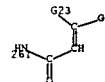


37

G2 = F  
G3 = alkyl <containing 1-3 C> (substd. by 1 or more G2)  
G6 = 64



G21 = 261



Patent location: claim 4  
Note: also incorporates claims 6, 10, 13 and 16

L23 ANSWER 9 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 141:7114 MARPAT Full-text  
TITLE: Preparation of benzoxazole, benzothiazole and benzimidazole acid derivatives for the treatment of cancer  
INVENTOR(S): Courtney, Stephen Martin; Hay, Philip Andrew; Scopes, David Ian Carter  
PATENT ASSIGNEE(S): Oxford Glycosciences (UK) Ltd., UK  
SOURCE: PCT Int. Appl., 64 pp.  
CODEN: PIXX02  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046122	A2	20040603	WO 2003-GB4991	20031117
WO 2004046122	A3	20040715		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RM: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TO

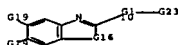
AU 2003283597 A1 20040615 AU 2003-283597 20031117

PRIORITY APPL. INFO.: GB 2002-26820 20021116  
GB 2003-19542 20030820

38

AB Title compds. I [R1-3 = H, halo, CF3, etc.; R4 = amido, aminosulfonyl, etc.; one of X, Y = COOH, tetrazole, etc.; Z = (un)substituted amino, O, S] are prepared. For instance, [3-(3-nitrobenzoylamino)-4-hydroxyphenyl]acetic acid Me ester (preparation given) is cyclized to the corresponding benzoxazoleacetic acid Me ester (PhMe, TsOH, reflux), reduced (dioxane, H2-10% Pd/C), acylated with 4-bromobenzoic chloride (THF, polymer-bound morpholine) and the resulting ester saponified (THF, LiOH) to give II. Selected compds. exhibit inhibition of heparanase and angiogenesis; I are useful for the treatment of cancer.

MSTR 1



G1 = phenylene (opt. substd.)  
G8 = NH  
G10 = carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd. by 1 or more F)  
G11 = 273

G10-G25

G16 = S  
G23 = 281

G16-G21

G26 = 166-10 167-282

G16-G21

Patent location: claim 1  
Note: or pharmaceutically acceptable salts, esters or prodrugs  
Note: also incorporates claims 12 and 17  
Note: substitution is restricted

L23 ANSWER 10 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 140:406811 MARPAT Full-text  
TITLE: Preparation of 6H-anthra[9,1-cd]isothiazol-6-one

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derivatives for treating inflammatory conditions or inhibiting JNK  
INVENTOR(S): Sakata, Steven T.; Raymon, Heather K.  
PATENT ASSIGNEE(S): Signal Pharmacapeutics, LLC, USA  
SOURCE: U.S. Pat. Appl. Publ., 60 pp., Cont.-in-part of U.S. Ser. No. 71,390.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004092562	A1	20040513	US 2003-407107	20030404
US 2003073732	A1	20030417	US 2002-71390	20020207
US 6987184	B2	20060117		
US 2006004080	A1	20060105	US 2005-159592	20050622
			US 2001-269013P	20010215
			US 2002-71390	20020207

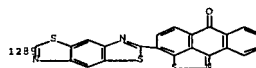
AB The title (un)substituted compds. I [wherein R = O, S, SO, SO2, or CH2] or deriva. or pharmaceutically acceptable salts thereof are prepared as Jun N-terminal kinase (JNK) inhibitors. For example, 1-aminoanthraquinone was reacted with NH4SCN in DMSO to give II. II showed inhibitory activity with IC50 of >30000 nM against enzymes p38-2 and MEK6. I are useful for the treatment of types I and II diabetes, obesity, etc. (no data).

MSTR 1



G2 = 37 / 1289

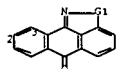
G2-G27



G10 = carbon chain <containing 1-8 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd. by G11)  
G11 = NH2

40

G27 = 3-71 2-70



G52 = 46

G10(10)

Patent location: claim 1  
Note: additional substitution also claimed

L23 ANSWER 11 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 140:391201 MARPAT Full-text  
TITLE: Preparation of 2-[2-(phenylamino)ethylamino]pyridine derivatives as inhibitors of glycogen synthase kinase 3  
INVENTOR(S): Nuss, John M.; Subramanian, Sharadha; Wagnan, Allan S.  
PATENT ASSIGNER(S): Chiron Corporation, USA  
SOURCE: PCT Int. Appl., 76 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037791	A1	20040506	WO 2003-US33370	20031020
WO 2004037791	B1	20040708		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2503819	A1	20040506	CA 2003-2502819	20031020
AU 2003282976	A1	20040513	AU 2003-282976	20031020
US 2004138273	A1	20040715	US 2003-690497	20031020
US 6989382	B2	20060124		
EP 1556355	A1	20050727	EP 2003-774908	20031020
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1717391	A	20060104	CN 2003-80104572	20031020
JP 20060506383	T	20060223	JP 2004-546978	20031020

41

LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035522	A1	20040429	WO 2003-JP11056	20030829
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2496633	A1	20040429	CA 2003-2496633	20030829
AU 2003261834	A1	20040504	AU 2003-261834	20030829
EP 1547996	A1	20050629	EP 2003-608871	20030829
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005260124	A1	20051124	US 2005-524691	20050215

PRIORITY APPL. INFO.:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002-255013			20020830	
JP 2002-255014			20020830	
JP 2002-255015			20020830	
JP 2003-73344			20030318	
WO 2003-JP11056			20030829	

AB Disclosed are compds. such as benzoxazole, benzothiazole, benzimidazole, quinoline, pyridine, benzene, thiazole, imidazole, pyrrole, furan, and benzoxazole derivs. represented by the general formula (I) or (II) or salts or solvates thereof [wherein D = NR', S, O, CH, CH<sub>2</sub>; wherein R' = H, C1-4 alkyl, halo-C1-4 alkyl, Ph, R, N, CH<sub>2</sub>, Q = N, CR<sub>2</sub>, R<sub>2</sub>, R<sub>1</sub>, R<sub>2</sub> = H, C1-4 alkyl, halo, HO, hydroxy-C1-4 alkyl, C1-4 alkoxy-C1-4 alkyl, NH<sub>2</sub>, C1-4 alkylamino, di(C1-4 alkyl)amino, NO<sub>2</sub>, C1-4 alkoxy, CO<sub>2</sub>H, SO<sub>3</sub>H, halo-C1-4 alkyl; m = an integer of 0-4; or R1 and R2 together form each (un)substituted benzene or naphthalene ring; R3 = groups listed for R<sub>1</sub>, R<sub>2</sub>, R<sub>1</sub>, or R<sub>2</sub>, Q-Q3, NHOR<sub>4</sub>; wherein R<sub>4</sub> = groups listed for R<sub>1</sub>, R<sub>2</sub>, R<sub>1</sub>, or R<sub>2</sub>, N-CH-allyl; A = R4-Q1, thiazole-2,4-diyl, oxazole-2,4-diyl, etc.; R<sub>5</sub> = groups listed for R<sub>1</sub>, R<sub>2</sub>, R<sub>1</sub>, or R<sub>2</sub>; X, Y = N, CH; Z = O, S, CH<sub>2</sub>, N-CpH<sub>2</sub>p+1; wherein p = an integer of 0-4] which are useful in the diagnosis, prevention, and/or treatment of diseases such as prion diseases or transmissible spongiform encephalopathies (TSEs) with accumulation of prion protein or in specific staining of prion protein contained in a specimen for imaging by PET or SPCT using positron or γ-ray emitting radionuclides. For example, 2-[2-(4-fluorophenyl)ethenyl]benzoxazole and 2-[2-(4-methylaminophenyl)ethenyl]quinoline inhibited the abnormal prion protein in mouse neuroblastoma ScN2a cells infected with sheep scrapie (sheep prion) with IC50 of 0.8 nM.

MSTR 1

G1-----G11-G17 G15

G1 = 8

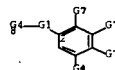
43

PRIORITY APPL. INFO.:

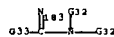
US 2002-420432P 20021021  
WO 2003-US33370 20031020

AB The title compds. I [wherein X and Y = independently N, O, and (un)substituted carbon; A1 and A2 = independently (un)substituted aryl, arylamino, aryloxy, or heteroaryl; R1-R4 = independently H, OH, (un)substituted alkyl, cycloalkyl, etc.; R1'-R4' = independently H or (un)substituted alkyl; R5-R7 = independently H, OH, halo, CO<sub>2</sub>H, NO<sub>2</sub>, amino, etc.] or pharmaceutically acceptable salts thereof are prepared as glycogen synthase kinase 3 (GSK3) inhibitors. For example, 2-(2,4-dichlorophenyl)-4-fluoro-1-nitrobenzene (preparation given) was reacted with 2-[[2-(aminoethyl)amino]-5-nitropyridine in MeCN in the presence of i-Pr<sub>2</sub>NH<sub>2</sub> to give I1 (90%). Some of compds. I showed inhibitory activity with IC50 of 1 μM or less against human GSK3. I are useful for the treatment of disorders mediated by GSK3 activity, such as for the treatment of diabetes, Alzheimer's disease, other neurodegenerative disorders, such as Parkinson's disease, Huntington's disease, obesity, atherosclerotic cardiovascular disease, essential hypertension, polycystic ovary syndrome, syndrome X, ischemia, traumatic brain injury, bipolar disorder, immunodeficiency, or cancer (no data).

MSTR 1



G4 = benzothiazolyl  
G7 = 183



G33 = alkyl (containing 1-10 C)  
(opt. substd. by 1 or more G24)

Patent location: claim 1  
Note: and pharmaceutically acceptable salts  
Note: substitution is restricted  
Note: additional ring formation also claimed

L23 ANSWER 12 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 140:352748 MARPAT Full-text  
TITLE: Heterocyclic compounds for use as diagnostic probes and remedies for diseases with accumulation of prion protein, and stains for prion protein  
INVENTOR(S): Doh-ura, Katsumi; Kudo, Yukitsuka; Sawada, Tohru  
PATENT ASSIGNER(S): SF Research Institute, Inc., Japan  
SOURCE: PCT Int. Appl., 128 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent

42



G2 = S  
G3 = N  
G5 = F  
G6 = 286-9 287-7



G17 = 178

WY=C(O)-G18

G18 = alkyl (containing 1-4 C)  
(opt. substd. by 1 or more G5)

G21 = phenylene (opt. substd.)  
Patent location: claim 1  
Note: or solvates

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 13 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 140:4955 MARPAT Full-text  
TITLE: Preparation of N-acylaminocetonitriles for controlling parasites  
INVENTOR(S): Ducray, Pierre; Goebel, Thomas; Bouvier, Jacques; Durano, Corinne  
PATENT ASSIGNER(S): Novartis Ag, Swiss; Novartis Pharma GmbH  
SOURCE: PCT Int. Appl., 64 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003097036	A1	20031127	WO 2003-EP5334	20030521
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC,				

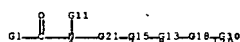
44

SE, SG, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW  
 RM: AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE,  
 DK, EE, ES, FI, FR, GB, GR, HU, IS, IT, LU, MC, NL, PT, RO, SE,  
 SI, SK, TR  
 CA 2483286 A1 20031127 CA 2003-2483286 20030521  
 AU 2003242555 A1 20031202 AU 2003-242555 20030521  
 BR 2003011214 A 20050301 BR 2003-11214 20030521  
 EP 1509221 A1 20050302 EP 2003-752774 20030521  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IS, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 CN 1649579 A 20050803 CN 2003-809965 20030521  
 US 2005182127 A1 20050818 US 2003-513806 20030521  
 JP 2005536466 T 20051202 JP 2004-505035 20030521  
 NZ 536184 A 20061027 NZ 2003-536184 20030521  
 CH 2002-855 20020522  
 WO 2003-EP5334 20030521

## PRIORITY APPLN. INFO.:

AB The title compds. [I; A1, A2 = (un)substituted aryl, heteroaryl, etc.; A3 = (un)substituted pyrimidinyl, s-triazinyl, 1,2,4-triazinyl, etc.; R1 = H, alkyl, haloalkyl, allyl, alkoxyalkyl; R2-R6 = H, halo, alkyl, etc.; or R2 and R3 are jointly alkylene; W = O, S, SO2, NR7; X = O, S, NR7; R7 = H, alkyl; a = 1-4; b = 0-4; c = 0-1] which have advantageous pesticidal properties, and are particularly suitable for controlling parasites in warm-blooded animals, were prepared and formulated. E.g., a multi-step synthesis of the benzamide II, starting from chloroacetone and 2-bromo-4,5-difluorophenol, was given.

## MSTR 1



G11 = CH2CH=CH2  
 G13 = bond  
 G15 = NH  
 G18 = phenylene (opt. substd. by 1 or more G32)  
 G21 = 5-4 6-7



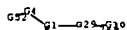
G24 = alkylene <containing 1 or more C> (opt. substd.)  
 G30 = benzothiazolyl  
 Patent location: claim 1

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 14 OF 34 MARPAT COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 139:292242 MARPAT Full-text

4; p = 0-3], were prepared. Thus, reaction of 3-F3CC6H4CHBrCO2Et with 2-(2-benzoxazolyl)-4-trifluoromethylphenol followed by saponification with LiOH gave title compound (III). III effectively lowered glucose in mice at 525 mg/kg orally.

## MSTR 1



G1 = NH  
 G4 = 20  
 G17 = alkyl <containing 1-8 C> (opt. substd. by 1 or more G18)  
 G18 = F  
 G29 = phenylene (opt. substd. by (up to 3) G37)  
 G30 = 369



G49 = S  
 Patent location: claim 1

L23 ANSWER 15 OF 34 MARPAT COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 139:218955 MARPAT Full-text  
 TITLE: Synthesis of phenylamino derivatives of benzothiazole, benzoxazole and indazole for use as sunscreens  
 INVENTOR(S): Dilk, Erich; Johncock, William; Langner, Roland  
 PATENT ASSIGNER(S): Haarmann & Reimer GmbH, Germany  
 SOURCE: Ger. Offen., 30 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10206562	A1	20030828	DE 2002-10206562	20020218
PRIORITY APPLN. INFO.:				
DE 2002-10206562 20020218				

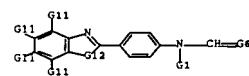
TITLE: Preparation of heteroarylphenoxyphenylacetates for treating diseases associated with glucose metabolism, lipid metabolism and insulin secretion.  
 INVENTOR(S): Zhao, Zuchun; Chen, Xin; Wang, Jianchao; Sun, Hongbin; Liang, Jack Shih-Chieh  
 PATENT ASSIGNER(S): Metabolex, Inc., USA  
 SOURCE: PCT Int. Appl., 330 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080545	A2	20031002	WO 2003-US8899	20030319
WO 2003080545	A3	20040122		
W: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KR, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IS, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
IN 2004DN03020	A	20070105	IN 2004-DN3020	20011004
CA 2479338	A1	20031002	CA 2003-2479338	20030319
AU 2003237787	A1	20031008	AU 2003-237787	20030319
US 2004029933	A1	20040212	US 2003-394487	20030319
US 7078421	B2	20060718		
EP 1487843	A2	20041222	EP 2003-736445	20030319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IS, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008537	A	20050209	BR 2003-8537	20030319
JP 2005520858	T	20050714	JP 2003-578306	20030319
CN 1653073	A	20050810	CN 2003-811039	20030319
NO 2004004436	A	20041206	NO 2004-4436	20041019
US 2006264630	A1	20061123	US 2006-326616	20060104
PRIORITY APPLN. INFO.:				
US 2002-366961P 20020320				
US 2003-394487 20030319				
WO 2003-US8899 20030319				

AB Title compds. [I, II; X = O, S, SO2, NR; R = H, alkyl, CO2R, CO2Ra, CONRbRb; Rb = H, alkyl; Y = CH2ORc, CO2Rc, CHO, CONRcRc, CH(NRc), CH(NORc), carboxylic acid surrogates; Rc = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, alkylene-2; Z = CORd, CO2Rd, NRdRe, NRdCONRrRr, NRdCORs, NRdCO2Re, CONRdRe; Rd, Re, Rf = H, alkyl, Ph; 2 of Rd, Re, Rf attached to the same N form a 5-6 membered ring; Rm = H, alkyl, aryl, OH, SO2Rn; Rn = alkyl, haloalkyl, aralkyl, heteroalkyl, aryl, heteroaryl, alkoxy, aryloxy, (di)alkylamino, (di)arylamino, haloalkylamino, di(haloalkyl)amino; RmRcn = 5-6 membered ring; Ar = (substituted) heteroaryl; q = 0-2; R1, R3 = halo, OH, alkyl, alkenyl, alkynyl, alkoxy, cycloalkyl, cycloalkylalkyl, haloalkyl, heteroalkyl, heterocyclyl, heterosubstituted cycloalkyl, heteroalkyl substituted cycloalkyl, haloalkoxy, NO2, cyano, Ph, PhO, NRj-Ph, SO2-Ph, CORj, CO2Rj, NRjRk, SO2RjRk, NRjCONRkRi, NRjCORk, NRjCORk, CONRjRk wherein the Ph ring is optionally substituted and Rj, Rk, Rl = H, alkyl, haloalkyl; 2 of Rj, Rk, Rl when attached to the same N form a 5-6 membered ring; r = 0-2; R2 = H, alkyl, haloalkyl, aralkyl, alkylene-2; m = 0-

AB The invention concerns the synthesis of phenylamino derivs. of benzothiazole, benzoxazole and indazole with the general formula (I), where Z = NH, O or S; R groups are defined; the products are used as sunscreens. Other sunscreens can be added. Thus [(N-methyl-N-(4-(6-methyl-1H-benzothiazol-2-yl)phenylamino)methylene]-propanedioic acid bis(2-ethylhexyl) ester was synthesized and included in a composition as a 3 weight/weight% ingredient; other components were (weight/weight%): Crodafores MCA 1.50; Cutina MD 2.00; Copherol 1250 0.50; Lanette 16 1.00; Tegosoft TN 24.00; Prisorine 3505 1.00; water 59.6; Tetrasodium EDTA 0.20; glycerin (99%) 3.00; phenoxyethanol 0.70; Solbrol M 0.20; Solbrol P 0.10; Carbolipol RTD 2050 0.20; sodium hydroxide (10% aqueous solution) 2.70; perfume 0.30.

## MSTR 1



G1 = alkyl <containing 1-20 C> (opt. substd. by 1 or more G2)  
 G2 = alkyl <containing 1-6 C> / CO2H (opt. substd.) / CONH2 (opt. substd.)  
 G6 = 44

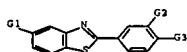


G7 = NH2  
 G10 = carbon chain <containing 1-20 C, 0 or more double bonds, no triple bonds> (opt. substd.)  
 G12 = S  
 Patent location: claim 1

L23 ANSWER 16 OF 34 MARPAT COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 139:193733 MARPAT Full-text  
 TITLE: Benzothiazole derivatives for in vivo imaging of amyloid plaques  
 INVENTOR(S): Wilson, Ian; Luthra, Sajinder Kaur; Brady, Frank  
 PATENT ASSIGNER(S): Amerham PLC, UK; Imaging Research Solutions Ltd.  
 SOURCE: PCT Int. Appl., 28 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE  
 WO 2003068269 A1 20030821 WO 2003-GB584 20030212  
 W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TO  
 CA 2474411 A1 20030821 CA 2003-2474411 20030212  
 AU 2003212490 A1 20030904 AU 2003-212490 20030212  
 EP 1474178 A1 20041110 EP 2003-708309 20030212  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, SE, HU, SK  
 US 2005123477 A1 20050609 US 2003-504231 20030212  
 JP 2005523903 T 20050811 JP 2003-567449 20030212  
 GB 2002-3391 20020212  
 GB 2002-17713 20020731  
 WO 2003-GB584 20030212  
 PRIORITY APPLN. INFO.:  
 AB The invention provides use of a compound of formula (I): or a salt thereof, wherein: R1 is 125I, 124I, 123I, 75Br, 76Br, or 18F; R2 is C1-6 alkyl; and R3 is selected from hydrogen, C1-6 alkyl, -C(O)C1-6 haloalkyl, and -C(O)CH(R4)NH2; wherein R4 is selected from hydrogen, C1-6 alkyl, C1-6 hydroxyalkyl, and C1-6 aminoalkyl, for the manufacture of a radiopharmaceutical for the in vivo diagnosis or imaging of an amyloid-associated disease, particularly Alzheimer's disease. As example, the preparation, biodistribution, pharmacokinetics, brain uptake, and amyloid binding of 5-[125I]-iodo-2-(4'-amino-3'-methylphenyl)benzothiazole are presented.

MSTR 1



G3 = 25

G5 = 4

G4 = alkylcarbonyl &lt;containing 1-6 C&gt;

(opt. substd. by 1 or more G5)

G5 = 7

Patent location: claim 1

Note: or salts

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MSTR 1



G4 = alkyl &lt;containing 1-20 C&gt;

(opt. substd. by 1 or more G5)

G5 = CN

G6 = 17

G7 = 4

G7 = NH

G9 = 63



Patent location: claim 1  
 Note: additional ring formation also claimed  
 Note: also incorporates claims 2, 3, 5, 7, 10, 11, and 13

L33 ANSWER 18 OF 34 MARPAT COPYRIGHT 2007 ACS ON STM  
 ACCESSION NUMBER: 137:93747 MARPAT Full-text  
 TITLE: Preparation of pyrazolecarboxamides as inhibitors of factor Xa  
 INVENTOR(S): Zhu, Bing-yan; Jia, Zhaozhong; Jon; Huang, Wenrong; Song, Yonghong; Kauter, James; Scarborough, Robert M.  
 PATENT ASSIGNER(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 303 pp., Cont.-in-part of U.S. Ser. No. 662,807.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 6  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003091116	A1	20020711	US 2001-794214	20010228
US 6632815	B2	20031014		
US 6720317	B1	20040413	US 2000-662807	20000915
US 6686368	B1	20040203	US 2003-387927	20030312
US 2004116399	A1	20040617	US 2003-600695	20030620

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REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT  
 L23 ANSWER 17 OF 34 MARPAT COPYRIGHT 2007 ACS ON STM  
 ACCESSION NUMBER: 138:212600 MARPAT Full-text  
 TITLE: Electroluminescent derivatives of 2,5-Diamino-terephthalic acids and their use in organic light-emitting diodes  
 INVENTOR(S): Richter, Andreas M.; Schoenewerk, Jens; Diener, Gerhard  
 PATENT ASSIGNER(S): Syntec Gesellschaft fuer Chemie und Technologie der Informationsaufzeichnung m.b.H., Germany  
 SOURCE: Ger. Offen., 34 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10141266	A1	20030306	DE 2001-10141266	20010821
WO 2003019697	A2	20030306	WO 2002-DE3110	20020821
WO 2003019697	A3	20031224		

W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TO  
 AU 2002325807 A1 20030310 AU 2002-325807 20020821  
 EP 1421634 A2 20040526 EP 2002-760128 20020821  
 EP 1421634 B1 20051116

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, SE, HU, SK  
 CN 1545741 A 20041110 CN 2002-816467 20020821  
 JP 2005500666 T 20050106 JP 2003-523038 20020821  
 AT 310320 T 20051215 AT 2002-760128 20020821  
 US 2005003230 A1 20050106 US 2004-487138 20040220  
 US 7112674 B2 20060926 US 2004-784149 20040220  
 US 2005025992 A1 20050203  
 US 7141312 B2 20061128

PRIORITY APPLN. INFO.:  
 DE 2001-10141266 20010821  
 WO 2002-DE3110 20020821

AB Organic electroluminescent devices are described which are provided with emitting layers comprising (un)doped compds. described by the general formula I (X1, X3 = independently selected atoms or groups including O, S, and imino groups; X2, X4 = independently selected atoms or groups including O, S, or (un)substituted amino groups; R1-8 = independently selected substituents including H, and C1-20 alkyl, aryl, or heteroaryl groups which may be further substituted; R4 and R8 may also be independently selected substituents chosen from halo, cyano, nitro, and amino groups; and rings may be formed between adjacent X and R groups).

50

US 2006020039 A1 20060126 US 2005-35767 20050114  
 PRIORITY APPLN. INFO.:  
 US 1999-154332P 19990917  
 US 2000-662807 20000915  
 US 2000-185746P 20000229  
 US 2000-663420 20000915  
 US 2001-794214 20010228

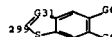
AB The title compds. AQDEGJX [A = alkyl, cycloalkyl, (un)substituted Ph, naphthyl, etc.; Q = a direct link, divalent alkyl, alkenyl, etc.; D = a direct link, (un)substituted Ph, 5-10 membered (non)aromatic heterocyclyl; S = a direct link, (CH2)qCO, CO(CH2)x, etc.; q, x = 0-2; G = (un)substituted Ph, 5-6 membered heteroaryl; J = a direct link, SO2, CO, etc.; X = (un)substituted Ph, naphthyl, 6-membered heteroaryl, etc.] having activity against mammalian factor Xa, and useful in vitro or in vivo for preventing or treating coagulation disorders, were prepared e.g., a 3-step synthesis of the pyrazolecarboxamide I was given.

MSTR 1C

G9-G10

G1 = phenylene (opt. substd.)

G2 = 299



G8 = (0-2) CH3

G9 = 21

G11-G12

G10 = alkyl &lt;containing 1-6 C&gt;

G11 = 65-2 66-22



G31 = N

Patent location: claim 1

Note: and all pharmaceutically acceptable salts, hydrates, solvates and prodrug derivative  
 Note: additional ring formation also claimed  
 Note: substitution is restricted

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## Stereochemistry:

and all pharmaceutically acceptable isomers

L23 ANSWER 19 OF 34 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:6177 MARPAT Full-text  
 TITLE: Preparation of phenylbenzimidazoles as osteoclast differentiation induction inhibitors and osteoclast inhibitors  
 INVENTOR(S): Nakahira, Hiroyuki; Horiuchi, Yoshihiro  
 PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 87 pp.  
 CODEN: JKXXAP  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002161084	A	20020604	JP 2000-360964	20001128
PRIORITY APPLN. INFO.:			JP 2000-360964	20001128

AB The compds. I [ring A, ring B = (un)substituted aromatic ring; X = NRO, S, O; RO = H, lower alkyl; Y = NR1R2, CONR1'R2', C(OH)R1'R2'', (un)substituted (un)saturated 5- to 7-membered heterocycle; R1 = (un)substituted lower alkyl, alkenyl, alkynyl; R2 = organic group excluding lower alkyl; R1R2 may form heterocycle; R1', R2' = (un)substituted lower alkyl; R1'R2'' may form heterocycle; R1'', R2'' = (un)substituted lower alkyl] or their pharmaceutically acceptable salts are prepared. The compds. are useful for anti-inflammatory agents, antirheumatic agents, and agents for bone regeneration. 2-(5,6-Dichloro-1H-imidazol-2-yl)-N-methylaniline (2.06 g) was reacted with acetyl chloride in pyridine at 25° for 1 h to give 630 mg N-(2-(5,6-dichloro-1H-benzimidazol-2-yl)phenyl)-N-methylacetamide showing 66% inhibition of osteoclast differentiation in vitro.

## MSTR 1



G1 = 98-4 99-6



G2 = 88-1 87-3

53

G3 = S  
G5 = 9G6 = Me  
G7 = 74

75(0)-G23-G26

G22 = alkyl (containing 1-6 C) (opt. substd.)  
G23 = 56

G26 = 77

G28 = CH  
Patent location: claim 1  
Note: or pharmaceutically acceptable salts

L23 ANSWER 20 OF 34 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:369706 MARPAT Full-text  
 TITLE: Preparation of benzoxazole LPAAT-β inhibitors  
 INVENTOR(S): Bonham, Lynn; Leung, David W.; Hollenbeck, David M.; Klein, J. Peter; Finney, Robert S.; White, Thayer H.; Shaffer, Scott A.; Tang, Norina M.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: PCT Int. Appl., 102 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

54

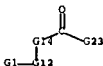
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002036580	A2	20020510	WO 2001-US42836	20011030
WO 2002036580	A9	20030213		
WO 2002036580	A3	20020906		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002016649 A5 20020515 AU 2002-16649 20011030  
 US 2002107269 A1 20020808 US 2001-984889 20011031  
 PRIORITY APPLN. INFO.: US 2000-244194P 20001031  
 WO 2001-US42836 20011030

AB The title compds. [I; R1 = halo, aryl, (un)substituted alkyl, alkoxy, aryloxy, substituted NH2; R2, R3 = H, halo, alkenyl, alkynyl, (un)substituted aryl, substituted NH2; provided that at least one of R2 and R3 = alkylacyl substituted NH2], useful in inhibiting lysophosphatidic acid acyltransferase β (LPAAT-β) activity, were prepared. Thus, reacting 3-(benzoxazol-2-yl)-4-chlorophenylamine (preparation given) with propionyl chloride in the presence of pyridine in THF afforded 100% I (R1 = H; R2 = 2-Cl; R3 = 5-(NHCOCH2Me)) which showed IC50 of 900 nM in LPAATβ colorimetric assay. The invention further relates to methods of treating cancer using benzoxazoles I. The invention also relates to methods for screening for LPAAT-β activity.

## MSTR 1



G1 = 63



G12 = phenylene (opt. substd. by (1) G13)  
 G14 = NH  
 G16 = carbon chain (containing 1-10 C, 0 or more double bonds, 0 or more triple bonds) (opt. substd.)  
 G17 = 40

55

G18 = F  
G23 = 111

111-016

Patent location: claim 15  
Note: or pharmaceutically acceptable salts or prodrugs  
Note: substitution is restricted

L23 ANSWER 21 OF 34 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:102232 MARPAT Full-text  
 TITLE: Preparation of 7-substituted tetracycline derivatives for pharmaceutical use as antibacterial agents  
 INVENTOR(S): Nelson, Mark L.; Frechette, Roger; Viskl, Peter; Ismail, Mohamed; Bower, Todd; Shatia, Beena; Messersmith, David; McIntyre, Laura; Kozs, Darrell; Rennie, Glen; Sheehan, Paul; Hawkins, Paul; Verma, Atul; Marchol, Tad; Bandarage, Upul  
 PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.  
 SOURCE: PCT Int. Appl., 97 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004407	A2	20020117	WO 2001-US20766	20010629
WO 2002004407	A3	20020404		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2415718 A1 20020117 CA 2001-2415718 20010629  
 AU 200171642 A 20020121 AU 2001-71642 20010629  
 AU 2001271642 B2 20060105  
 US 2003055025 A1 20030320 US 2001-895812 20010629  
 US 6818635 B2 20041116  
 EP 1301466 A2 20030416 EP 2001-950674 20010629  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 BR 2001012265 A 20030624 BR 2001-12265 20010629  
 HU 200301163 A2 20030828 HU 2003-1163 20010629

56

Patent location: claim 1  
Note: and pharmaceutically acceptable salts

PATENT NO.	KIND DATE		APPLICATION NO.	DATE
WO 2001019798	A2	200101022	WO 2000-0525195	200009315
WO 2001019798	A3	200101025		
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PK, PL, PT, RU, SA, SD, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KR, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SF, SJ, CP, CO, CI, CM, GA, GN, GW, ML, MR, NE, NU, TD, TO				
CA 2385589	A1	200101022	CA 2000-235589	20000915
AU 200074866	A	200104177	AU 2000-74866	20000915
US 5176123	B2	20050612		
EP 1216231	B2	20020626	EP 2000-963451	20000915
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IS, SI, LT, LV, FI, RO, MK, CY, AL				
BR 2000014078	A	20021231	BR 2000-14078	20000915
TR 200201413	T2	20030321	TR 2002-1413	20000915
JP 2003059412	T	20030311	JP 2001-523378	20000915
HU 200203954	A2	20030328	HU 2002-3954	20000915
US 5176123	A	200101031	US 2000-517628	20000915
WO 2002001230	A	20020511	WO 2002-1230	20020312
ZA 2002003117	A	20031315	ZA 2002-2117	20020314
ZA 2002002116	A	20040210	ZA 2002-2116	20020314
ZA 2003006488	A	20040216	ZA 2003-6488	20030220
ZA 2003006490	A	20040323	ZA 2003-6490	20030220
US 2006020039	A1	200606126	US 2005-35767	20050114
RITY APPLN. INFO.: US 1999-154322P 19990917				
US 2000-185766P 20000929				
US 2000-663420 20000915				
WO 2000-0525195 20000915				

AB The title compds. ADDQBXJ, [A = alkyl, cycloalkyl, (un)substituted Ph; Q = a direct link, alkylene, CO, etc.; D = a direct link, (un)phenylene, etc.; E = a direct link, (CH<sub>2</sub>)<sub>Q</sub>CO, SO<sub>2</sub>, etc.; Q = 0-2; G = (un)substituted Ph, (un)substituted 5-6 membered (non)aromatic heterocyclic a ring containing 1-4 heteroatoms selected from N, O and S; J = a direct link, SO<sub>2</sub>, CO, etc.; X = (un)substituted Ph, naphthyl, heterocycle having activity against mammalian factors Xa, and thrombin. More useful *in vitro* or *in vivo* for preventing or treating coagulation disorders I was described. E.g., a 3-step synthesis of the purgazolecarboxamide I was described.

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G17	= N	
G32	= CH2	
Patent location:		claim 1
Note:		substitution is restricted
Note:		additional ring formation also claimed
Note:		additional combinations of groups in G8 and G9 also claimed
Note:		or pharmaceutically acceptable salts, hydrates, solvates and prodrug derivatives
Stereochemistry:		or pharmaceutically acceptable isomers

L23 ANSWER 23 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 133:335167 MARPAT Full-text  
TITLE: Preparation of diaryl carboxylic acids and derivatives  
as peroxisome proliferator-activated receptor ligands.  
INVENTOR(S): Janyosi, Zaid; McGehee, Gerard M.; Kelley, Michael  
F.; Lebaudun, Ronald; Grancher, Lita; Gronsberg,  
Robert D.; McGarry, Daniel G.; Caulfield, Thomas J.;  
Minnich, Anne; Bobko, Mark  
PATENT ASSIGNEE(S): Aventis Pharmaceuticals Products Inc., USA  
SOURCE: PCT Int. Appl., 167 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent

LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000064888	A1	2000020105	WO 2000-US911833	20000428
M: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, ES, ES, FI, GB, GR, GR, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LU, LV, MA, MG, MK, MN, MX, MY, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UG, UZ, VN, ZA, ZW				
RM: GH, GM, GR, LS, MW, GD, SL, SZ, TZ, UZ, YN, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IR, IT, LU, MC, NL, PT, SE, SF, BJ, CF, CG, CI, CM, GA, GN, GW, HE, IL, LR, NM, NE, SD, TD, TG				
CA 2370280	A1	200001102		20000428
EP 177187	A1	20000206	EP 2000-932698	20000428
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010605	A	20000213	BR 2000-10605	20000428
AU 200001291	A2	200002928	AU 2002-1291	20000428
BR 200000556	B1	20000217	BR 2000-556	20000428
NZ 515086	A	20010311	NZ 2000-515086	20000428
AU 781266	B2	20000512	AU 2000-46895	20000428
RU 2267484	C	200006110	RU 2001-132080	20000428
US 6635655	B1	20031021	US 2000-662649	20000914
MO 2001005075	A	20011123	MO 2001-5075	20011018
ZA 200100798	B	20030305	ZA 2001-0798	20011024
HR 2001000795	A1	20030228	HR 2001-795	20011026
PRIORITY APPLN. INFO.:			US 1999-134155P	19990428

AB Ar1(CR1R3)A(CR3R4)baR2(CR5R6)c(CR7R8)dR2A(CR9)U-Us1R3Us2 70000478  
 Ar1 = aryl, CR1 = aryl, CR2 = alkyl, CR3 = aryl, CR4 = aryl, CR5 = aryl,  
 arylcycloalkenyl, fused arylcycloalkyl, fused arylheterocycloalkenyl, fused  
 arylheterocycyl, heteroaryl, fused heteroaryl, cycloalkenyl, fused  
 heteroaryl, cycloalkyl, fused heteroaryl, heterocycyl, etc.; A = O, S, SO, SO2,  
 NR13, CO, NR14CO, CONR15, NR14CONR15, CR14=N, bond, etc.; B = O, S, NR19,  
 bond, CO, NR20CO, CONR20; S = bond, CH2CH2; Z = R21O2C, R21OC, cycloimide,  
 cyano, R21O2CSN, R21O2SN, (R21)NCO, R21O-substituted, 2,  
 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, R2, R5, R7 = H,  
 halo, alkyl, CO2H, alkoxycarbonyl, arylalkyl; R2, R4, R6, R8 = (CH2)q; q = 0-3;  
 R14, R15, R20 = H, alkyl, aralkyl, CO, alkoxycarbonyl; R14R15 = atoms to form  
 a 5-6 membered azaheterocycyl; R19, R21 = H, aryl, alkyl, cycloalkyl,  
 aralkyl). were prepared as agonists or antagonists of the PPAR receptor (no  
 data). Thus, 3-(quinolin-2-ylmethoxy)propan-1-ol in DMPP/THF at 0° was  
 treated with 2-benzoyl-2-benzoyl-2-benzoyl-2-benzoylbenzoate by  
 stirring overnight at room temperature to give Me 2-methyl-6-[3-(quinolin-2-  
 ylmethoxy)propoxy]methylbenzoate.

G1 = benzothiazolyl  
G2 = 2-1 3-4 / phenylene

G3-G14

G3 = 5-1 6-3 / 7-1 8-3 / 9-1 11-3

G4-G5 G5-G6 G5-G1-G5

G5 = carbon chain (containing 1 or more C,  
0 or more double bonds, no triple bonds) (opt. substd.)

G16 = 58 / 401

G17-G18 (O)-G17 G17-G18

G17 = NH2 (opt. substd.)

G18 = 355-60 356-59 / 357-60 358-59 / 359-60 361-59

G19-G20 G19-G21 G19-G22

G19 = NH (opt. substd.)

G21 = 403-60 404-402 / 405-60 406-402 /  
407-60 409-402

G22-G23 G22-G24 G22-G25

Patent location: claim 1

Note: additional ring formation and substitution also claimed

Note: or pharmaceutically acceptable salts, N-oxides, hydrates or solvates

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 24 OF 34 MARPAT COPYRIGHT 2007 ACS ON STM

ACCESSION NUMBER: 133:321881 MARPAT [Full-text](#)

TITLE: Preparation of bisbenzoxoles as antineoplastic agents.

INVENTOR(S): Heidle, Stephen; Mann, John

PATENT ASSIGNEE(S): University of Reading, UK; Institute of Cancer Research; Queen's University of Belfast

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

61

10/511,852

April 27, 2007

INVENTOR(S): Sato, Koichi; Mori, Yoshimasa; Haniu, Yukio; Shinjo, Kensei; Nakamura, Shinichi; Yamada, Shuji; Noguchi, Koji

PATENT ASSIGNEE(S): Canon K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 70 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 10213820 A 19980811 JP 1997-19315 19970131

PRIORITY APPLN. INFO.: JP 1997-19315 19970131

AB In the component containing a chiral smectic liquid crystal between a pair of substrates having electrodes and orientation-controlling layers, the liquid crystal has 22 stable states and several layer structures in driving chiral smectic phases and shows ratio of apparent tilt angle to intrinsic tilt angle 20.5 and anisotropy of dielec. constant  $\Delta\epsilon(-1)$ . The device using the component is also claimed. The component gives high-contrast and large-area display devices.

MSTR 1

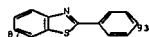
G1-G2-G3-G4-G5-G6

G1 = pentyl

G2 = bond

G5 = NH

G6 = 87-2 93-4



Patent location: claim 2

Note: substitution is restricted

L23 ANSWER 26 OF 34 MARPAT COPYRIGHT 2007 ACS ON STM

ACCESSION NUMBER: 128:277024 MARPAT [Full-text](#)

TITLE: Photographic element containing improved couplers

INVENTOR(S): Edwards, James Lawrence; Lau, Philip T. S.; Cowan, Stanley Wray

PATENT ASSIGNEE(S): Eastman Kodak Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 46 pp.

CODEN: JKKXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

63

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2000063180 A1 20001026 WO 2000-GB1479 20000417

M: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CP, CO, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1173422 A1 20020123 EP 2000-920882 20000417

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

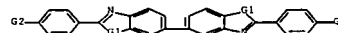
US 5589971 B1 20030708 US 2003-959084 20020418

PRIORITY APPLN. INFO.: GB 1999-5828 19990416

WO 2000-GB1479 20000417

AB Title compds. [I; X1, X2 = NH, O, S; A1, A2 = YQZ, LM; Y = O, NH, S; Q = (CH2)n, C3-7 carbocyclyl; n = 0-10; Z = H, amino, heterocyclyl; l = linking group; M = alkylating agent functionality], were prepared. Thus, 4,4'-diamino-3,3'-dinitrobiphenyl was hydrogenated in acetone over Raney Ni and the residue was heated with 4-(3-dimethylamino-1-propoxy)benzaldehyde in PhNO2 at 150° for 12 h to give 35% I [X1, X2 = NH; R2 = O(CH2)3NMe2]. This showed IC50 = 0.235 μM against A2780 cells, vs. 12.0 μM for Hoechst 33258.

MSTR 1



G1 = NH / S

G2 = 65

G3-G4-H

G9 = G10

G10 = (1-10) CH2

Patent location: claim 1

Note: or pharmaceutically acceptable salts or tautomers

Note: substitution is restricted

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 25 OF 34 MARPAT COPYRIGHT 2007 ACS ON STM

ACCESSION NUMBER: 129:182166 MARPAT [Full-text](#)

TITLE: Chiral smectic liquid-crystal component and high-contrast liquid-crystal device using it

62

10/511,852

April 27, 2007

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 10083048 A 19980331 JP 1997-224080 19970820

US 5888716 A 19990330 US 1996-699904 19960820

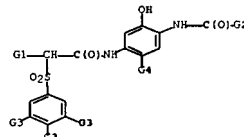
GB 2316495 A 19980225 GB 1997-17322 19970818

GB 2316495 B 20000906

PRIORITY APPLN. INFO.: US 1996-699904 19960820

AB The title element comprises a red-sensitive Ag halide emulsion layer containing a cyan dye-forming coupler I (R1 = H or alkyl; R2 = alkyl or aryl; n = 1-3; X = alkyl, alkenyl, alkoxy, aryloxy, acyloxy, acylamino, sulfonyloxy, sulfamoylamino, sulfonamido, ureido, oxycarbonyl, oxycarbonylamino or carbamoyl which is at the m- or p-position to the sulfonyl group; Z = H or group releasing upon coupling with oxidized color developing agents) and a green-sensitive Ag halide emulsion layer containing a magenta dye-forming coupler II or III (Z = H or coupling-releasing group; R1d, R1f = H or substituent). The cyan coupler promotes the increase in green and blue chromaticness.

MSTR 1



G1 = 109

F2-G2-F2

G4 = benzothiazolyl

Patent location: claim 1

L23 ANSWER 27 OF 34 MARPAT COPYRIGHT 2007 ACS ON STM

ACCESSION NUMBER: 128:45575 MARPAT [Full-text](#)

TITLE: Preparation of fluorescent group-containing carbodiimide compounds for nucleic acid detection

INVENTOR(S): Suzuki, Osamu; Masuda, Gen; Shiohata, Mamiko; Matsumoto, Kazuko

PATENT ASSIGNEE(S): Nissinbo Industries, Inc., Japan; Nissinbo Spinning

SOURCE: Eur. Pat. Appl., 50 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

64

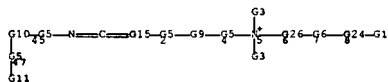


LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 808829	A1	19971126	EP 1997-303430	19970520
EP 808829	B1	20030409		
JP 10287870	A	19981027	JP 1997-122638	19970513
JP 3851706	B2	20061129		
US 5856479	A	19990105	US 1997-857536	19970516
			JP 1996-124793	19960520
			JP 1996-296887	19961108
			JP 1997-32459	19970217

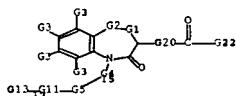
PRIORITY APPLN. INFO.:  
AB Fluorescent group-containing carbodiimides are prepared for use in the detection of nucleic acids by immuno- or chemiluminescence assays. Thus, 1-aminopyrene and 3-(dimethylamino)propyl isothiocyanate to give a thiourea followed by conversion to the title carbodiimide. The above compound was used for the detection of hybrid nucleic acid.

MSTR 1B



AB Title compds. [I; A = (un)substituted alkylene; R = (CH<sub>2</sub>)<sub>q</sub>LR<sub>7</sub>; L = (un)substituted divalent benzo-fused heterocyclyl; R<sub>1</sub>, R<sub>2</sub> = H, halo, (perfluoro)alkyl, Ph, etc.; R<sub>4</sub>, R<sub>5</sub> = H, alkyl, Ph, etc.; R<sub>6</sub> = H, alkyl, phenyl(alkyl); R<sub>7</sub> = (un)substituted Ph; X = CO, O, SOO-2, CH(OH), CH=CH, etc.; n = 0 or 1; p = 0-3; q = 0-4] were prepared as growth hormone release promoters (no date). Thus, 1-tetralone was converted in 5 steps to 3(R)-amino-2,3,4,5-tetrahydro-1H-benzazepin-2-one which was amidated by H<sub>2</sub>OCCCH<sub>2</sub>Me<sub>2</sub>NHBOC (preparation given) to give benzazepinylaminoalkanamide II (R = H, R<sub>5</sub> = BOC) which was N-alkylated by BrCH<sub>2</sub>LR<sub>7</sub> (CH<sub>2</sub>LR<sub>7</sub> = benzofuranylmethyl group O, R<sub>9</sub> = trityl-protected 5-tetrazolyl) to give, after deprotection, II (R = O, R<sub>5</sub> = H, R<sub>9</sub> = 5-tetrazolyl).

## MSTR 1A



G1 = (0-3) CH<sub>2</sub>  
G5 = 137-15 142-17

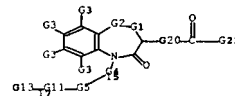


G6 = S  
G11 = phenylene  
G13 = 346



G14 = alkyl <containing 1-10 C>  
(opt. substd. by (1-3) G15)  
G15 = alkoxy-carbonyl <containing 1-5 C> / CO<sub>2</sub>H  
Derivative: and pharmaceutically acceptable salts  
Patent location: claim 1

## MSTR 1A



G1 = (0-3) CH<sub>2</sub>  
G5 = 137-15 142-17



G6 = S  
G11 = phenylene  
G13 = 346



G14 = alkyl <containing 1-10 C>  
(opt. substd. by (1-3) G15)  
G15 = alkoxy-carbonyl <containing 1-5 C> / CO<sub>2</sub>H  
Derivative: and pharmaceutically acceptable salts  
Patent location: claim 1

L23 ANSWER 31 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 120:311502 MARPAT Full-text  
TITLE: Electrophotographic photoreceptor containing enamine compound  
INVENTOR(S): Enomoto, Kazuhiro; Kondo, Akihiro; Kurokawa, Makoto; Masuda, Akiko; Machino, Masaru  
PATENT ASSIGNEE(S): Sharp KK, Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.  
CODEN: JXXXXP  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05323636	A	19931207	JP 1992-128979	19920521
JP 2790396	B2	19980827		

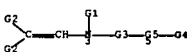
PRIORITY APPLN. INFO.: JP 1992-128979 19920521

69

70

AB The photoreceptor contains an enamine compound (charge-transporting agent) having a general structure I [R = Cl -4 alkyl, alkenyl, (substituted) aryl, aralkyl, heterocyclyl; A, B = H, Cl -4 alkyl, (substituted) heterocyclyl, aryl; X = (substituted) arylene; Y = S, O, Se; Z = hydrocarbon (forming a 5-membered ring with N and V); n = 0, 1]. The enamine compound may be represented by II. The photoreceptor shows high sensitivity and durability.

## MSTR 1



G1 = Ph  
G2 = alkyl <containing 1-4 C>  
G3 = phenylene  
G4 = 16



G5 = (0-1) CH=CH  
G6 = S  
Patent location: claim 1

L23 ANSWER 32 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 120:137094 MARPAT Full-text  
TITLE: Preparation of azo dyes  
INVENTOR(S): Raue, Roderich; Lange, Karl  
PATENT ASSIGNEE(S): Bayer A.-G., Germany  
SOURCE: Ger. Offen., 19 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4242428	A1	19931028	DE 1992-4242428	19921215
EP 567849	A1	19931103	EP 1993-106056	19930414
JP 06049375	A	19940222	JP 1993-116631	19930421
US 5541299	A	19960730	US 1994-311831	19940923
US 5502171	A	19960326	US 1995-442049	19950516
US 5578711	A	19961126	US 1995-527971	19950914
			US 1992-874674	19920427
			DE 1990-4008263	19900315

PRIORITY APPLN. INFO.:

71

US 1991-665632 19910306  
DE 1992-4242428 19921215  
US 1993-48024 19930415  
US 1994-311831 19940923  
US 1995-442049 19950516  
AB Triazene and triazatrimethine dyes XN:NY (X = aromatic or heterocyclic group; Y = arylamino or heterocyclic imino group) are prepared from the resp. aromatic or heterocyclic diazo component and arylamino or heterocyclic imine coupling component by coupling under 5-100 bars CO<sub>2</sub> pressure in the presence of a HNO<sub>2</sub> acid-releasing substance at 0-125° in aqueous medium. Thus, 2-amino-5-(diisopropylamino)-1,3,4-thiadiazole, 2-amino-3-methylbenzothiazolium Me sulfate, and isoamyl nitrite in aqueous MeOH were kept 3 h at 40° under 50 bars CO<sub>2</sub> pressure and the product was treated with Me<sub>2</sub>SO<sub>4</sub> to give a cationic dye which provided lightfast red shades on acrylic fibers.

## MSTR 3



G2 = 23



G6 = 115



G7 = 25



G8 = alkyl <containing 1-8 C>  
(opt. substd. by 1 or more G26)  
G21 = phenylene  
G22 = benzothiazolyl  
G26 = CN / 144



Patent location: claim 1

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L23 ANSWER 33 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 116:22880 MARPAT Full-text  
 TITLE: Triphenodioxazine dyes, their preparation and use  
 INVENTOR(S): Jaeger, Horst  
 PATENT ASSIGNEE(S): Bayer A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 27 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 448815	A1	19911002	EP 1990-124689	19901219
EP 448815	B1	19940928		
R: CH, DE, FR, GB, LI				
DE 4010223	A1	19911002	DE 1990-4010223	19900330
US 5202436	A	19930413	US 1991-666092	19910307
JP 04224869	A	19920814	JP 1991-84452	19910326
JP 2941990	B2	19990830		

PRIORITY APPLN. INFO.: DE 1990-4010223 19900330  
 AB The dyes (I; R = H, (un)substituted C1-6-alkyl; R1 = H, substituent; R2, R3 = H, Cl, Br, (un)substituted alkyl, alkoxy, Ph, or phenoxy; R4 = cleavable group; R5 = aryl, optionally with an azo linkage; n = 0, 1) are prepared and used to dye cellulosic fibers, wool, silk, and synthetic polyamides. Thus, 0.1 mol 3,10-diamino-6,13-dichlorotriphenodioxazine-4,11-disulfonic acid was treated with 0.1 mol cyanuric chloride and then 0.1 mol 4-amino-N-(4-sulfonyl)benzamide to give I [R = R1 = H; R2 = R3 = R4 = Cl; R5 = 4-(4-sulfoanilino)carbonyl)phenyl; n = 1; SO3H in 4- and 11-positions], clear blue on cotton.

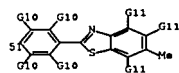
MSTR 40

H—q2—G9

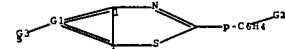
G2 = 33

H—G1

G3 = alkyl (containing 1-6 C)  
 (opt. substd. by 1 or more G4)  
 G4 = alkyl (containing 1-4 C)  
 G9 = S1



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G1 = 10-1 13-3 10-5



G2 = 26



G5 = 58



G8 = 62-26 63-59



G9 = OMe  
 G17 = alkylene  
 Patent location: claims  
 Note: record may include structures from disclosure

Patent location: claim 3

L23 ANSWER 34 OF 34 MARPAT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 102:158128 MARPAT Full-text  
 TITLE: Two component diazo material  
 INVENTOR(S): Scheler, Siegfried  
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 47 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3307364	A1	19840906	DE 1983-3307364	19830302
ES 529801	A1	19850316	ES 1984-529801	19840216
EP 118086	A2	19840912	EP 1984-101944	19840224
EP 118086	A3	19870527		
EP 118086	B1	19890927		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 46773	T	19891015	AT 1984-101944	19840224
DK 8401054	A	19840903	DK 1984-1054	19840227
NO 8400758	A	19840903	NO 1984-758	19840228
JP 59165050	A	19840918	JP 1984-35467	19840228
US 4540648	A	19850910	US 1984-584547	19840228
CA 1211977	A1	19860930	CA 1984-448420	19840228
FI 8400810	A	19840903	FI 1984-810	19840229
FI 74825	B	19871130		
FI 74825	C	19880310		
ZA 8401513	A	19841031	ZA 1984-1513	19840229
BR 8400996	A	19841009	BR 1984-996	19840301
PRIORITY APPLN. INFO.: DE 1983-3307364 19830302				
EP 1984-101944 19840224				

AB A 2-component diazo copying material having a flat gradation and that can be used for the reproduction of halftone originals without any appreciable loss in copying speed contains a support coated with a photosensitive layer containing a diazonium salt, a coupler, an acid stabilizer, and a salt of a benzothiazole derivative (I; R = H, alkyl, or aryl; R1 = H, or optionally substituted alkyl, aralkyl, aryl, pyridylalkyl, carbalkyl, carboxyalkyl, carboxyaryl, carbamoyl, or sulfamoyl, or R1 and R2 together form a heterocyclic ring; R2 = H or alkyl) that absorbs in the UV region and upon treatment with an alkaline medium is converted to a nonabsorbing leuco base form. Thus, a glass-clear PET support was coated with a composition containing cellulose acetate propionate 14.00, Me2CO 135.00, MeOH 35.00, Me glycol 8.00, BuOH 8.00, 5-sulfoisocyclohexanecarboxylic acid 0.41, 2-hydroxy-3-naphthoic acid N-(2-methoxyphenyl) amide 0.88, 1-hydroxy-2-naphthoic acid N-piperidine 0.60, 2,5-diethoxy-4-N-morpholinobenzene diazonium tetrafluoroborate 1.56 g, and 6-methyl-2-(4-aminophenyl)benzothiazole 10 weight% (based on the above diazonium salt), dried 1 min at 100°, exposed, and processed to show an effect copying speed of 71% and a clear flattening of the gradation.

MSTR 1

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## INVENTOR NAME SEARCH

=> fil heap medline embase biosis wpi  
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L24 2687 SEA WAGNER B/AU OR WAGNER B ?/AU OR WAGNER BARB?/AU  
 L25 62 SEA ("EHLIS T"/AU OR "EHLIS THOMAS"/AU)  
 L26 25 SEA ("MONJAT S"/AU OR "MONJAT SEBASTIEN"/AU OR "MONJAT SEBASTIEN"/AU)  
 L27 13 SEA ("RICHIN K"/AU OR "RICHIN K H"/AU OR "RICHIN KAI"/AU)  
 L28 8 SEA (L24 AND (L25 OR L26 OR L27)) OR (L25 AND (L26 OR L27)) OR (L26 AND L27)  
 L29 3 SEA (L24 OR L25 OR L26 OR L27) AND ?BENZOTHAZOL  
 L30 9 SEA L28 OR L29

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L30 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2006:34174 HCAPLUS Full-text  
 DOCUMENT NUMBER: 144:134682  
 TITLE: Preparation of merocyanine derivatives for UV protection formulations  
 INVENTOR(S): Wagner, Barbara; Bienenwald, Frank; Wollieb, Helms; Wallquist, Olof; Herzog, Bernd; Ehlig, Thomas; Heese, Jürg  
 PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Swiss.  
 SOURCE: PCT Int. Appl., 66 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006003094	A2	20060112	WO 2005-EP52850	20050620
WO 2006003094	A3	20060713		
M: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BO, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MX, MY, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,				

ZA, ZM, ZW  
 RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
 IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF,  
 CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BM, GH, GM,  
 KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO,  
 KZ, MD, RU, TJ, TM  
 GB 2416351 A 20060125 GB 2005-12335 20050617  
 EP 1761237 A 20070314 EP 2005-756874 20050620  
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
 IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR  
 PRIORITY APPLN. INFO.: EP 2004-103018 A 20040629  
 WO 2005-EP52850 W 20050620

OTHER SOURCE(S): MARPAT 144:134682  
 AB Disclosed are the preparation and use such as for protecting of human hair and skin against the damaging effect of UV radiation of merocyanine derivate. An example compound I was prepared from dehydroacetic acid and DMP di-Me acetate. I and three other compds. were formulated into UV protection lotions.

L30 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2005:535935 HCAPLUS Full-text  
 DOCUMENT NUMBER: 143:83167  
 TITLE: Merocyanine derivatives as sunscreens and UV absorbers for cosmetic use  
 INVENTOR(S): Wagner, Barbara; Ehlig, Thomas; Mueller, Stefan  
 PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.  
 SOURCE: Brit. UK Pat. Appl., 101 pp.  
 CODEN: BAXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2409203	A	20050622	GB 2004-27078	20041210
AU 2004298775	A1	20050630	AU 2004-298775	20041208
WO 200508269	A1	20050630	WO 2004-EP53327	20041208
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: BW, GR, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1701695	A1	20060920	EP 2004-820463	20041208
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1897911	A	20070117	CN 2004-8003827	20041208
BR 2004017827	A	20070410	BR 2004-17827	20041208
PRIORITY APPLN. INFO.:			EP 2004-104746	A 20031217
			EP 2004-102155	A 20040517
			WO 2004-EP53327	W 20041208

OTHER SOURCE(S): MARPAT 143:83167

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AB Cosmetic compns. comprising a merocyanine derivative are described as sunscreens for protecting human and animal hair and skin from UV radiation. Methods for preparation of merocyanine derivate, as well as intermediates with UV absorbing properties are also described. The compns. further comprise an addnl. UV absorber selected from triazine compds. Thus, a mixture of 9.06 g diisodone and 2.78 g piperazine in toluene was heated under reflux conditions for 5 h. After cooling down the mixture, the product (compound MCo6a) was filtered off, washed and dried (yield 75%). Di-Me sulfate (3.34 g) was added dropwise to 4.33 g of the compound MCo6a and the mixture was stirred for 60 min at 100°. After cooling down to 80°, a mixture of 2.89 g Et cyanoacetate and 5.21 g of triethylamine was added dropwise. The reaction mixture was stirred at a temperature of 110° for 90 min. After cooling down and the addition of 300 mL water, the raw product (compound MCo7; I) was filtered off, purified by column chromatog. and dried. The I absorption maximum  $\lambda_{max}$  in ethanol was 406 nm. The merocyanine derivate were used in preparation of skin-care formulations together with other UV absorbers, e.g., ethylhexyl methoxycinnamate, Uvinul A Plus or benzylidene camphor.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2004:515467 HCAPLUS Full-text  
 DOCUMENT NUMBER: 141:71355  
 TITLE: Preparation of amino substituted hydroxyphenyl benzophenone derivatives as UV absorbers  
 INVENTOR(S): Haase, Juerg; Ehlig, Thomas; Boreas, Elek; Mueller, Stefan  
 PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.  
 SOURCE: PCT Int. Appl., 50 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052837	A2	20040624	WO 2003-EP50937	20031203
WO 2004052837	A3	20040910		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: BW, GR, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003298343	A1	20040630	AU 2003-298343	20031203
EP 1569893	A2	20050907	EP 2003-796081	20031203
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
BR 2003016607	A	20051011	BR 2003-16607	20031203
CN 1726184	A	20060125	CN 2003-80105885	20031203
JP 20060509834	T	20060323	JP 2005-502323	20031203
US 2006014846	A1	20060126	US 2005-537940	20050607
PRIORITY APPLN. INFO.:			EP 2002-406093	A 20031212
			CH 2003-1113	A 20030625
			EP 2003-102297	A 20030725

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OTHER SOURCE(S): MARPAT 141:71355  
 AB Disclosed are aminohydroxybenzophenonecarboxamide derivate of formula (I) [wherein R1, R2 = independently C1-30 alkyl, C2-20 alkenyl, C3-10 cycloalkyl, C1-10 C3-C10 cycloalkenyl; or R1 and R2 together with the linking nitrogen atom form a 5- or 6-membered heterocyclic ring; n1 = 1-4; when n1 = 1, R3 = saturated or unsatd. heterocyclic radical, hydroxy-C1-C5 alkyl, cyclohexyl optionally substituted with one or more C1-5 alkyl, Ph optionally substituted with a heterocyclic radical, aminocarboxyl, C1-5 alkylcarboxy; when n1 = 2, R3 = alkylene, cycloalkylene or alkenylene radical which is optionally substituted by a carbonyl or carboxy group; or R3 together with A forms a bivalent radical of the formula Q; wherein n2 = 1-3; when n1 = 3, R3 = alkanetriyl radical; when n1 = 4, R3 = alkanetetriyl radical; A = O, N(R5); R5 = H, C1-5 alkyl, hydroxy-C1-5 alkyl]. These compds. are useful as UV filters in sunscreen applications, preferably for the protection of human and animal hairs and from the damage of UV radiation as well as cosmetic compns. comprising these compds. Thus, a solution of 10.6 g 3-diethylaminodibenzoxepin (preparation given) in 20 mL diethylene glycol di-Me ether was added to a suspension of 7.2 g 2-(4-aminophenyl)-6-methylbenzothiazole are suspended in 60 mL diethylene glycol di-Me ether at room temperature under stirring, heated to 90°, and allowed to react for 4 h to give 7.3 g H-[4-(6-methylbenzothiazol-2-yl)phenyl]-2-(4-diethylamino-2-hydroxybenzoyl)benzamide.

L30 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2004:60279 HCAPLUS Full-text  
 DOCUMENT NUMBER: 140:116975  
 TITLE: Merocyanine derivatives used for sunscreen  
 INVENTOR(S): Wagner, Barbara; Ehlig, Thomas; Elschin, Kai  
 PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.  
 SOURCE: PCT Int. Appl., 74 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004006678	A1	20040122	WO 2003-EP6955	200310701
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: GR, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003250866	A1	20040202	AU 2003-250866	200310701
BR 2003012500	A	20050412	BR 2003-12500	200310701
EP 1494283	A1	20050706	EP 2003-763671	200310701
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1665475	A	20050907	CN 2003-816155	200310701
JP 20051215	J2	20051215	JP 2004-520442	200310701
IN 2004CN03070	A	20060217	IN 2004-CN3070	20041231

79

US 2005255055 A1 20051117 US 2005-520840 20050107  
 PRIORITY APPLN. INFO.: EP 2002-405582 A 20020710  
 WO 2003-EP6955 W 200310701

OTHER SOURCE(S): MARPAT 140:116975  
 AB Disclosure is the use of merocyanine derivate as sunscreen to protect human and animal hair and skin from UV radiation. For example, Et2NCH=CHCH(CN)CO2CH2CH2(R)2 was prepared and used in the skin-care formulation together with glyceryl stearate, stearic acid, cetyl alc. and polysorbate 20.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2003:836808 HCAPLUS Full-text  
 DOCUMENT NUMBER: 139:327911  
 TITLE: Aminophenyl-benzothiazole compounds as UV filters in cosmetics  
 INVENTOR(S): Wagner, Barbara; Ehlig, Thomas; Moogiat, Sebastian; Elschin, Kai  
 PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.  
 SOURCE: PCT Int. Appl., 48 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003086341	A2	20031023	WO 2003-EP3870	20030414
WO 2003086341	A3	20040401		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: GR, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003292665	A1	20031027	AU 2003-292665	20030414
EP 1494641	A2	20050112	EP 2003-722472	20030414
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
BR 2003009308	A	20050215	BR 2003-9308	20030414
CN 1646507	A	20050727	CN 2003-808638	20030414
US 2005175554	A1	20050811	US 2003-511852	20030414
JP 2005529869	T	20051006	JP 2003-583365	20030414
IN 2004CN02985	A	20070302	IN 2004-CN2985	20041117
PRIORITY APPLN. INFO.:			EP 2002-405311	A 20030417
			CH 2002-2135	A 20021216
			WO 2003-EP3870	W 20030414

OTHER SOURCE(S): MARPAT 139:327911  
 AB The preparation and use, as a UV filter, of a compound of formula I (R1, R2 = H, unsubstituted or halo-, amino-, mono- or di-C1-5-alkylamino-, cyano- or C1-5-alkoxy-substituted C1-22-alkyl, C5-10-cycloalkyl, carboxy-C1-22-alkyl, carboxy-C6-10-aryl, C6-10-aryl, C6-10-aryl-C1-5-alkyl; carbamoyl-, sulfinyl-, sulfonyl-, R1, R2, W forming 5- to 7-membered heterocyclic radical; R3 = H, C1-22-alkyl; R4 = H, OH, C1-22-alkyl, C1-22-alkoxy) is

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described. The compds. of formula I in micronized form are suitable as UV absorbers in cosmetic preps. and for protecting hair and skin from UV radiation.

L30 ANSWER 6 OF 9 WPX COPYRIGHT 2007 THE THOMSON CORP ON STN  
 ACCESSION NUMBER: 2006-079942 [08] WPX  
 DOC. NO. CPI: C2006-028367 [08]  
 TITLE: Use of merocyanine derivative as anti-wrinkle perception modifier to provide excellent protection of human skin against damaging effect of sunlight  
 DERIVAT CLASS: D21; E19  
 INVENTOR: BIENEMALD F; ENLIS T; HAASE J; HERZOG B; MAHNER B; WALLQUIST O; WOLLSEB H  
 PATENT ASSIGNEE: (CIBA-C) CIBA SPECIALTY CHEM HOLDING INC  
 COUNTRY COUNT: 110  
 PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2006003094	A2	20060112	(200608)	EN	66[0]	
GB 2416351	A	20060125	(200608)	EN		
EP 1761237	A2	20070314	(200722)	EN		

## APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2006003094	A2	WO 2005-EP52850	20050620
GB 2416351	A	GB 2005-12335	20050617
EP 1761237	A2	EP 2005-756874	20050620
EP 1761237	A2	WO 2005-EP52850	20050620

## FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1761237	A2	Based on
		WO 2006003094

PRIORITY APPLN. INFO: EP 2004-103018 20040629

AB WO 2006003094 A2 UPAB: 20060331

NOVELTY - A merocyanine derivative is used as an anti-wrinkle perception modifier.

DETAILED DESCRIPTION - Use of merocyanine derivative of structure (1) as anti-wrinkle perception modifier.

Q-H, 1-22C alkyl, -OR, -OR7, -NR7R8 or -N-R9;  
 R1-H; 1-22C alkyl; -OR7, -SR7, -NR7R8; 2-12C alkyl, 2-12C alkenyl; 2-12C alkynyl; 3-12C cycloalkyl; 3-22C cycloalkenyl; 7-12C aralkyl; 1-12C heteroalkyl, 2-11C heteroalkenyl; 6-10C aryl; or 1-9C heteroaryl;  
 R4-cyano; COR7, COOR7; CONR7R8, SO2(6-12C)aryl; 2-12C alk-1-enyl; 3-12C cycloalk-1-enyl; 2-12C alk-1-ynyl; 2-12C heteroalkyl; 3-5C heterocycloalkyl; 6-10C aryl; or 1-9C heteroaryl;  
 R5-COR7, -COOR7; -OR7, -SR7, -NR7R8; 1-2C alkyl; 2-12C alkenyl; 2-12C alkynyl; 3-12C cycloalkyl; 3-12C cycloalkenyl; 7-12C aralkyl; 1-12C alkylphenyl; 1-12C alkoxy-6-10C aryl; 1-12C heteroalkyl; 2-11C heteroalkenyl; 3-12C cycloheteroalkyl; 6-10C aryl; 1-12C alkoxy-6-10C aryl; or 1-9C heteroaryl;  
 R6-H; 1-22C alkyl; 1-22C alkoxy; or COR7;

R7 and R8-H; 1-22C alkyl; 2-12C alkenyl; 2-12C alkynyl; 3-12C cycloalkyl; 3-12C cycloalkenyl; -(CH2)COOH; 7-12C aralkyl; 1-12C heteroalkyl; 2-11C heteroalkenyl; 6-10C aryl; 1-9C heteroaryl; Si-R10R11R12; Si(OR10)(OR11)(OR12); Si-R10(OR11OR12); SiR10R11(OR12); -(CH2)u-O-(CH2)v-SiR10R11R12; or a radical X-Si1;

T, u and v=1-5;  
 R9=1-6C alkylidene radical;  
 R10-R12=1-22C alkyl;  
 X-linker:  
 Si1=silane-, oligosiloxane- or polysiloxane radical;  
 n=1-4.

R1 and R2, R1 and Q, R1 and R6, R1 and T, R2 and R3, R2, R4, R2, R6, R2 and Q R4 R1 or R2, R1 and Q, R1 and R6, R1 and T, R6 and Q, T and Q are linked together, so that 1, 2, 3 or 4 carboxylic or N, O and/or S-heterocyclic rings are formed, where each of them, independently from each other, may be condensed with an aromatic or heteroaromatic ring, and/or more N-, O- and/or S-heterocyclic rings, and each N atom in a N-heterocyclic ring may be substituted by 1-22C alkyl.

At least one of the radicals R1, R6 or Q is different from hydrogen, that if n=1 T=CO2R5; -CN; 6-10C aryl; -NHR5; or -SO2-6-12C)aryl; R2 and R3=1-22C alkyl; hydroxy-1-22C alkyl; 2-12C alkenyl; 2-12C alkynyl; 3-12C cycloalkyl, 3-12C cycloalkenyl; 7-12C aralkyl; 1-12C heteroalkyl; 3-12C cycloheteroalkyl; 6-10C aryl; 1-9C heteroaryl; or a radical of structure (1a);  
 p=5-100;  
 q=1-5;

n=0-4; if n=2;  
 R2 and R3=1-6C alkylene; and simultaneously T is defined as for n=1;  
 or T=bivalent radical of structure -NR7-V-NR7-;  
 V=phenylene; or 1-5C alkylene;  
 R7=H or 1-5C alkyl; and R2 and R3=defined as for n=1; if n=3, one of R2, R3 or T=trivalent radical; if n=4 one of R2, R3 or T is a tetravalent radical; for protecting of human hair and skin against the damaging effect of UV radiation.

An INDEPENDENT CLAIM is included for an ultraviolet absorber dispersion comprising micronized absorber each having a particle size of 0.02-2 microns; and dispersing agent.

USE - The merocyanine derivative is used as anti-wrinkle perception modifier (claimed). It is also used as ultraviolet filters, i.e. for protecting ultraviolet-sensitive organic materials in particular the skin and hair of humans and animals from harmful effects of radiation. It is also used as sunscreens in cosmetics preparation, pharmaceutical and veterinary medical preparations.

ADVANTAGE - The invented merocyanine derivative provides excellent protection of human skin against the damaging effect of sunlight.

L30 ANSWER 7 OF 9 WPX COPYRIGHT 2007 THE THOMSON CORP ON STN  
 ACCESSION NUMBER: 2005-481205 [49] WPX  
 DOC. NO. CPI: C2005-146778 [49]  
 TITLE: Use of merocyanine compounds to protect human and animal hair and skin from UV radiation and intermediates for the preparation of UV absorbers  
 DERIVAT CLASS: D21; E19  
 INVENTOR: ENLIS T; MUELLER S; MAHNER B; MUELLER S  
 PATENT ASSIGNEE: (CIBA-C) CIBA SPECIALTY CHEM HOLDING INC; (CIBA-C) CIBA SPECIALTY CHEM HOLDING INC  
 COUNTRY COUNT: 107  
 PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
GB 2409203	A	20050622	(200549)	EN	101[0]	
WO 2005058269	A1	20050630	(200651)	EN		
EP 1701695	A1	20060920	(200662)	EN		
MX 2006006409	A1	20060901	(200706)	ES		
AU 2004298775	A1	20050630	(200707)	EN		

## APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
GB 2409203	A	GB 2004-27078	20041210
EP 1701695	A1	EP 2004-820463	20041208
WO 2005058269	A1	WO 2004-EP53327	20041208
EP 1701695	A1	WO 2004-EP53327	20041208
MX 2006006409	A1	WO 2004-EP53327	20041208
MX 2006006409	A1	MX 2006-6409	20060606
AU 2004298775	A1	AU 2004-298775	20041208

## FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1701695	A1	Based on
		WO 2005058269
MX 2006006409	A1	Based on
		WO 2005058269
AU 2004298775	A1	Based on
		WO 2005058269

PRIORITY APPLN. INFO: EP 2004-102155 20040517

AB GB 2409203 A UPAB: 20051223

NOVELTY - Use of merocyanine compounds (A) in protecting human and animal hair and skin from UV radiation.

DETAILED DESCRIPTION - Use of merocyanine compounds (A) of formulae (1a) and (1b) in protecting human and animal hair and skin from UV radiation.

R2 = H, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl or CN;  
 R4 = CN or -O1-R5;  
 Q = -COO-, -CONH-, -CO-, -SO2- or -CONR6-;  
 R5 = 1-22C alkyl, cyclo-3-8C alkyl or 1-6C alkyl-substituted-6-20C aryl;  
 R6 = H, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl;  
 cyclohexene radical C = substituted by one or more 1-5C alkyl; and n, o = 2-4.

In formula (1a):  
 Either R1 = alkylene, cycloalkylene or phenylene-radical; or R1=R2 = (cyclo)alkylene or phenylene; and either  
 R3 = CN or -O1-R5; or  
 R3=R4 = 5-7 membered or monocyclic carbocyclic ring (both optionally interrupted by -O- or -NR7-) (if n is 2).

In formula (1b):  
 R3 = (cyclo)alkylene or phenylene (both optionally substituted with 1-4C alkyl, 1-4C alkoxy, -COR6, -COOR6 or -CONR6); either  
 R1 = H, CN, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; or  
 NR1R2 = -(CH2)m- ring (optionally interrupted by -O- or -NR7-);  
 R7 = H, 1-2C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; and

m = 3-7 (if o is 2).  
 In formula (1a):  
 R1 = trivalent alkyl group (optionally interrupted by one or more -O- or -NR7-); and either  
 R3 = CN or -O1-R5; or  
 R3=R4 = 5-7 membered or monocyclic carbocyclic ring (if n is 3).  
 In formula (1b):  
 R3 = (cyclo)alkylidene or phenylidene radical; and either  
 R1 = H, CN, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; or  
 NR1R2 = -(CH2)m- ring (optionally interrupted by -O- or -NR7-) (if o is 3).  
 In formula (1a):  
 R1 = tetravalent alkyl group; and either  
 R3 = CN or -O1-R5; or  
 R3=R4 = 5-7 membered or monocyclic carbocyclic ring (if n is 4).  
 In formula (1b):  
 R3 = tetravalent alkyl group; and either  
 R1 = H, CN, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; or  
 NR1R2 = -(CH2)m- ring (optionally interrupted by -O- or -NR7-) (if n is 4).

INDEPENDENT CLAIMS are also included for:  
 (1) a cosmetic preparation comprising (A) with cosmetically acceptable carriers or adjuvants;  
 (2) phenyl compounds of formulae (a1) or (a2);  
 (3) use of a monomeric, oligomeric or polymeric compound comprising cyclohexene amine compounds of formula (2) as UV chromophores in protecting human and animal hair and skin from UV radiation; and  
 (4) 1,2-cyclohexen-3-one compounds of formula (3).

In formulae (a1-a2):  
 either R-2a = H, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl or CN; or  
 NR-1aR-2a = -(CH2)m- ring optionally interrupted by O or -NR-7a;  
 R-4a = -O-1a-R-5a;  
 Q-1a = -COO-, -CONH-, -CO-, -SO2- or -CONR6-;  
 R-5a = 1-22C alkyl, cyclo-3-8C alkyl or unsubstituted or 1-6C alkyl-substituted-6-20C aryl;  
 R-6a = H, 1-22C alkyl, cyclo-3-8C alkyl, unsubstituted or 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl;  
 R-7a = H, 1-22C alkyl, cyclo-3-8C alkyl, unsubstituted or 1-6C alkyl or 1-6C alkoxy-substituted-6-20C aryl;  
 cyclohexene radical C = not optionally substituted by one or more 1-5C alkyl;

n = 3-7;  
 n = 2-4; and  
 o = 2-4.  
 In formula (a1):  
 either R-1a = alkylene, cycloalkylene or phenylene-radical; or  
 R-1a-R-2a = (cyclo)alkylene or phenylene; and either  
 R-3a = CN or -O-1a-R-5a; or  
 R-3a-R-4a = 5-7 membered or monocyclic carbocyclic ring (if n is 2).  
 In formula (b1):  
 either R-3a = (cyclo)alkylene or phenylene; and either  
 R-1a = H, CN, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; or  
 NR-1aR-2a = -(CH2)m- ring (optionally interrupted by -O- or -NR-7a-) (if o is 2).  
 In formula (a1):

R-1a = trivalent alkyl group (optionally interrupted by one or more -O- or -NR-7a-); and either  
 R-3a = CN or -O-1a-R-5a; or  
 R-3a-R-4a = 5-7 membered or monocyclic carbocyclic ring (if n equals 3).  
 In formula (b1):  
 R-1a = (cyclo)alkylidene or phenylidene radical; and either  
 R-1a = H, CN, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; or  
 NR-1aR-2a = -(CH2)m- ring (optionally interrupted by -O- or -NR-7a-) (if n is 3).  
 In formula (a1):  
 R-1a = tetravalent alkyl group; and either  
 R3 = CN or -O-1a-R-5a; or  
 R-3a-R-4a = 5-7 membered or monocyclic carbocyclic ring (if n is 4).  
 In formula (b1):  
 R-3a = tetravalent alkyl group; and either  
 R-1a = H, CN, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl; or  
 NR-1aR-2a = -(CH2)m- ring (optionally interrupted by -O- or -NR-7a-) (if n is 4).  
 In formula (3):  
 R2 = H, 1-22C alkyl, cyclo-3-8C alkyl, 1-6C alkyl- or 1-6C alkoxy-substituted-6-20C aryl;  
 R3 = H, 1-22C alkyl, cyclo-3-8C alkyl or unsubstituted or 1-6C alkyl-substituted 6-20C aryl;  
 m = 3-7;  
 n = 2-4; and  
 cyclohexene radical C = not optionally substituted 1-5C alkyl.  
 Provided that when n is 2 and R1, R2 is simultaneously form (cyclo)alkylene or phenylene; when n is 3 and R1 is trivalent alkyl group is optionally interrupted by one or more -O- or -NR3-; and when n is 4 and R1 is tetravalent alkyl group which is optionally interrupted by one or more -O- or -NR3-.

USE - (A) are useful as UV-B absorbers in protecting human and animal hair and skin from UV radiation. (A) are useful as intermediates for the preparation of UV absorbers. (A) are also useful for the preparation of cosmetic (all claimed).  
 ADVANTAGE - (A) has poor oil-solubility and high melting point, which is suitable in particular as UV absorbers in the micronized state.

L30 ANSWER 8 OF 9 WPIC COPYRIGHT 2007 THE THOMSON CORP ON STN  
 ACCESSION NUMBER: 2004-143033 [14] WPIC  
 DOC. NO. CPI: C2004-057636 [14]  
 TITLE: Use of novel merocyanine derivative for cosmetics, for protecting human and animal hair and skin from ultraviolet radiation  
 DERIVAT CLASS: D21; E19  
 INVENTOR: EHLIS T; RICHIN K; WAGNER B  
 PATENT ASSIGNEE: (CIBA-C) CIBA SPECIALTY CHEM HOLDING INC; (EHLI-I) EHLIS T; (RICH-I) RICHIN K; (WAGN-I) WAGNER B; (CIBA-C) CIBA SC HOLDING AG  
 COUNTRY COUNT: 104  
 PATENT INFO ABBR.:  
 PATENT NO KIND DATE WEEK LA PG MAIN IPC  
 WO 2004006878 A1 20040122 (200414) \* EN 74 [0]

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10/511,852  
 AU 2003250866 A1 20040202 (200450) EN  
 BR 2003012500 A 20050412 (200526) PT  
 EP 1549283 A1 20050706 (200544) IN  
 KR 2005025342 A 20050314 (200557) KO  
 MX 2005000440 A1 20050401 (200571) ES  
 US 20050255055 A1 20051117 (200576) EN  
 JP 2005538072 W 20051215 (200582) JA 78  
 CN 1665475 A 20050907 (200607) ZH  
 IN 2004003070 P4 20060217 (200619) EN

## APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2004006878 A1		WO 2003-EP6955	20030701
AU 2003250866 A1		AU 2003-250866	20030701
BR 2003012500 A		BR 2003-12500	20030701
CN 1665475 A		CN 2003-816155	20030701
EP 1549283 A1		EP 2003-763671	20030701
BR 2003012500 A		WO 2003-EP6955	20030701
EP 1549283 A1		WO 2003-EP6955	20030701
MX 2005000440 A1		WO 2003-EP6955	20030701
US 20050255055 A1		WO 2003-EP6955	20030701
JP 2005538072 W		WO 2003-EP6955	20030701
JP 2005538072 W		JP 2004-520442	20030701
US 20050255055 A1		US 2005-520840	20050107
KR 2005025342 A		KR 2005-700480	20050110
MX 2005000440 A1		MX 2005-440	20050110
IN 2004003070 P4		WO 2003-EP6955	
IN 2004003070 P4		IN 2004-CN3070	20041231

## FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2003250866 A1	Based on	WO 2004006878 A
BR 2003012500 A	Based on	WO 2004006878 A
EP 1549283 A1	Based on	WO 2004006878 A
MX 2005000440 A1	Based on	WO 2004006878 A
JP 2005538072 W	Based on	WO 2004006878 A

## PRIORITY APPLN. INFO: EP 2002-405582 20020710

AB WO 2004006878 A1 UPAB: 20060320  
 NOVELTY - Novel merocyanine derivatives are used in protecting human and animal hair and skin from ultraviolet radiation.  
 DETAILED DESCRIPTION - Novel merocyanine derivatives of formulae (1), (2) or (3) are used in protecting human and animal hair and skin from ultraviolet radiation.  
 R1, R2, R5, R6 = H, 1-22C alkyl, 3-8C cyclo alkyl, or unsubstituted or 1-6C alkyl or 1-6C alkoxy substituted 6-20C aryl, and R1 and R2 combine with nitrogen atom and form -(CH2)m- ring which is (un)substituted by -O- or by -NH-;  
 R3 = cyano, -COOR5, -CONHR5, -COR5, -SO2R5, or -CONR1R5;  
 R4 = cyano, -COOR6, -CONHR6, -SO2R6, or -CONR2R6, and R3 and R4, or R5 and R6 together form a 5-7 membered, monocyclic, carbocyclic or heterocyclic ring;  
 Z1, Z2 = -(CH2)1 group which is (un)substituted by -O-, -S-, or -NR7- and/or (un)substituted 1-6C alkyl;  
 R7 = 1-5C alkyl;  
 1 = 1-4;

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m = 1-7; and  
 n = 1-4.  
 When n is 2, R1, R5, or R6 is bivalent alkyl, or R1 and R2 combined with 2 nitrogen atoms linking to form -(CH2)m- ring. When n is 3, R1, R5 or R6 is a trivalent alkyl group, and when n is 4, R1, R5 or R6 is a tetravalent alkyl group, and R1 and R2 in formula (1) are not hydrogen.  
 INDEPENDENT CLAIMS are included for the following:  
 (1) a cosmetic preparation comprising at least 1 or more compounds of formulae (1) or (2) along with cosmetically acceptable carriers or adjuvants; and  
 (2) a compound of formula (6).  
 R1 = 1-4C alkylene;  
 R2 = 1-5C alkyl, and R1 and R2 combined with nitrogen atoms to form -(CH2)m-;  
 R5 = 1-22C alkyl; and  
 m = 1-7.  
 USE - For cosmetics used for protecting human and animal hair and skin from ultraviolet radiation (claimed).  
 ADVANTAGE - The merocyanine compounds have ultraviolet absorbing property, and hence suitable for cosmetic formulations and pharmaceutical compositions.

L30 ANSWER 9 OF 9 WPIC COPYRIGHT 2007 THE THOMSON CORP ON STN  
 ACCESSION NUMBER: 2003-865305 [80] WPIC  
 DOC. NO. CPI: C2003-244687 [80]  
 TITLE: Use of aminophenylbenzothiazole compound as ultraviolet filter  
 DERIVAT CLASS: D21; E13  
 INVENTOR: EHLIS T; RICHIN K; MONGIAT S  
 PATENT ASSIGNEE: (CIBA-C) CIBA SC HOLDING AG; (CIBA-C) CIBA SPECIALTY CHEM HOLDING INC; (EHLI-I) EHLIS T; (RICH-I) RICHIN K; (MONG-I) MONGIAT S; (WAGN-I) WAGNER B  
 COUNTRY COUNT: 102  
 PATENT INFO ABBR.:  
 PATENT NO KIND DATE WEEK LA PG MAIN IPC  
 WO 2003086341 A2 20031023 (200380) \* EN 48 [0]  
 AU 2003229665 A1 20031027 (200436) EN  
 EP 1494641 A2 20050112 (200504) EN  
 BR 2003009308 A 20050215 (200517) PT  
 KR 2004108742 A 20041224 (200528) KO  
 US 20050175554 A1 20050811 (200553) EN  
 MX 2004009176 A1 20050101 (200564) ES  
 JP 2005529869 W 20051006 (200566) JA 48  
 CN 1646507 A 20050727 (200577) ZH

## APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2003086341 A2		WO 2003-EP3870	20030414
AU 2003229665 A1		AU 2003-229665	20030414
BR 2003009308 A		BR 2003-5308	20030414
CN 1646507 A		CN 2003-808618	20030414
EP 1494641 A2		EP 2003-722472	20030414
JP 2005529869 W		JP 2003-583365	20030414

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10/511,852  
 EP 1494641 A2  
 BR 2003009308 A  
 US 20050175554 A1  
 MX 2004009176 A1  
 JP 2005529869 W  
 KR 2004108742 A

## FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2003229665 A1	Based on	WO 2003086341 A
EP 1494641 A2	Based on	WO 2003086341 A
BR 2003009308 A	Based on	WO 2003086341 A
MX 2004009176 A1	Based on	WO 2003086341 A
JP 2005529869 W	Based on	WO 2003086341 A

## PRIORITY APPLN. INFO: CH 2002-2135 20021216

AB WO 2003086341 A2 UPAB: 20060203  
 NOVELTY - Aminophenylbenzothiazole compound is used as UV filter.  
 DETAILED DESCRIPTION - Use of aminophenylbenzothiazole compound formula (I) as an UV filter.  
 R1 and R2 = H, unsubstituted or halo-, amino-, mono- or di-(1-5)C alkylamino-, cyano- or 1-5C alkoxy-substituted 1-22C alkyl, 5-10C cycloalkyl, carboxy- 1-22C alkyl, carboxy-(6-10)C aryl, 6-10 aryl, 6-10C aryl-(1-5)C alkyl; carbamoyl; or sulfamoyl; or together with N atom form 5- to 7- membered heterocyclic radical;  
 R3 = or 1-22C alkyl; and  
 R4 = H, OH; 1-22C alkyl; or 1-22C alkoxy.  
 INDEPENDENT CLAIMS are also included for:  
 (a) a method of preparing of the compound of formula (I), comprising the alkylating R3-substituted 2-(4-aminophenyl)-benzothiazole with the appropriate haloalkane/haloalkane (R1-Hal and R2-Hal) using a base, according to reaction scheme (A) or (B); and  
 (b) a cosmetic preparation comprising the compound of formula (I) and carriers or adjuvants.  
 USE - (I) is used as UV filter (claimed). It is used for cosmetic or pharmaceutical preparations such as creams, gels, lotions, alcoholic and aqueous/alcoholic solutions, emulsions, wax/fat compositions, stick preparations, powders or ointments.  
 ADVANTAGE - The use of the aminophenylbenzothiazole compound provides excellent protection of human skin against the damaging effect of sunlight.

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## SEARCH HISTORY

&gt;&gt; d his nofil

(FILE 'HOME' ENTERED AT 12:37:02 ON 27 APR 2007)

FILE 'REGISTRY' ENTERED AT 12:37:25 ON 27 APR 2007

L1 48389 SEA ABB=ON PLU=ON "CARBAMOYL"

L2 46217 SEA ABB=ON PLU=ON L1 NOT MAN/CI

L3 5325 SEA ABB=ON PLU=ON L2 NOT RSD/FA

L4 715 SEA ABB=ON PLU=ON L3 AND C<5

L5 19831 SEA ABB=ON PLU=ON "SULFAMOYL"

L6 882 SEA ABB=ON PLU=ON L5 NOT MAN/CI AND C<6

L7 STR

L8 2 SEA SSS SAM L7

L9 D SCA

33 SEA SSS FUL L7

FILE 'HCAPLUS' ENTERED AT 12:57:15 ON 27 APR 2007

L10 13 SEA ABB=ON PLU=ON L9

E US2004-511852/APPS

E WO2003-EP3870/APPS

L11 1 SEA ABB=ON PLU=ON (WO2003-EP3870/AP OR WO2003-EP3870/PRN)

L12 1 SEA ABB=ON PLU=ON L11 AND L10

FILE 'BEILSTEIN' ENTERED AT 12:58:42 ON 27 APR 2007

L13 1 SEA SSS SAM L7

L14 8 SEA SSS FUL L7

L15 2 SEA ABB=ON PLU=ON L14 AND RN/FA

L16 6 SEA ABB=ON PLU=ON L14 NOT L15

L17 6 SEA ABB=ON PLU=ON L16 AND BABSAN/FA

SEL BABSAN L17

FILE 'BABS' ENTERED AT 12:59:38 ON 27 APR 2007

L18 2 SEA ABB=ON PLU=ON (6336258/BABSAN OR 6596140/BABSAN)

D BIB TOT

FILE 'HCAPLUS' ENTERED AT 13:00:00 ON 27 APR 2007

L19 4 SEA ABB=ON PLU=ON L10 AND PY=2002

L20 1 SEA ABB=ON PLU=ON L19 AND ANTITUMOR BENZOTHAZOL7/TI

D BIB

FILE 'MARPAT' ENTERED AT 13:01:23 ON 27 APR 2007

L21 2 SEA SSS SAM L7

L22 36 SEA SSS FUL L7

L23 34 SEA ABB=ON PLU=ON L22 NOT L10

FILE 'HCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 13:02:10 ON 27 APR 2007

L24 2687 SEA ABB=ON PLU=ON WAGNER B/AU OR WAGNER B 7/AU OR WAGNER BARB7/AU

E EHLIS T/AU

L25 62 SEA ABB=ON PLU=ON ("EHLIS T"/AU OR "EHLIS THOMAS"/AU)

E MONGIAT S/AU

L26 25 SEA ABB=ON PLU=ON ("MONGIAT S"/AU OR "MONGIAT SEBASTIEN"/AU OR "MONGIAT SEBASTIEN"/AU)

E RICHIN K/AU

L27 13 SEA ABB=ON PLU=ON ("RICHIN K"/AU OR "RICHIN K H"/AU OR "RICHIN KAI"/AU)

L28 8 SEA ABB=ON PLU=ON (L24 AND (L25 OR L26 OR L27)) OR (L25 AND (L26 OR L27)) OR (L26 AND L27)

L29 3 SEA ABB=ON PLU=ON (L24 OR L25 OR L26 OR L27) AND ?BENZOTHAZO L7

L30 9 SEA ABB=ON PLU=ON L28 OR L29

FILE 'HCAPLUS' ENTERED AT 13:04:37 ON 27 APR 2007

D QUE L10

D L10 IBIB ABS HITSTR TOT

FILE 'MARPAT' ENTERED AT 13:05:02 ON 27 APR 2007

D QUE L23

D L23 IBIB AB QHIT TOT

FILE 'HCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 13:10:07 ON 27 APR 2007

D QUE L30

D L30 IBIB AB TOT

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTARHH1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR 7):2

\*\*\*\*\* Welcome to STN International \*\*\*\*\*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
 NEWS 2 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals  
 NEWS 3 JAN 16 CA/Caplus Company Name Thesaurus enhanced and reloaded  
 NEWS 4 JAN 16 IPC version 2007.01 Thesaurus available on STN  
 NEWS 5 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data  
 NEWS 6 JAN 22 CA/Caplus updated with revised CAS roles  
 NEWS 7 JAN 22 CA/Caplus enhanced with patent applications from India  
 NEWS 8 JAN 29 PHAR reloaded with new search and display fields  
 NEWS 9 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases  
 NEWS 10 FEB 15 PATDPASP enhanced with Drug Approval numbers  
 NEWS 11 FEB 15 RUSSAPAT enhanced with pre-1994 records  
 NEWS 12 FEB 23 KORAPAT enhanced with IPC 8 features and functionality  
 NEWS 13 FEB 26 MEDLINE reloaded with enhancements  
 NEWS 14 FEB 26 EMBASE enhanced with Clinical Trial Number field  
 NEWS 15 FEB 26 TOXCENTER enhanced with reloaded MEDLINE  
 NEWS 16 FEB 26 IFICDB/IFIPAT/IFIUDS reloaded with enhancements  
 NEWS 17 FEB 26 CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases  
 NEWS 18 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
 NEWS 19 MAR 16 CASREACT coverage extended  
 NEWS 20 MAR 20 MARPAT now updated daily  
 NEWS 21 MAR 22 LMPI reloaded  
 NEWS 22 MAR 30 RDISCLOSURE reloaded with database clusters and STN  
 NEWS 23 APR 02 JICST-EPLUS removed from database clusters and STN  
 NEWS 24 APR 30 GRNBANK reloaded and enhanced with Genome Project ID field  
 NEWS 25 APR 30 CHEMCATS enhanced with 1.2 million new records  
 NEWS 26 APR 30 CA/Caplus enhanced with 1870-1889 U.S. patent records  
 NEWS 27 APR 30 INPADOC replaced by INPADOCDB on STN  
 NEWS 28 MAY 01 New CAS web site launched  
 NEWS 29 MAY 08 CA/Caplus Indian patent publication number format defined  
 NEWS 30 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
 NEWS 31 MAY 21 BIOSIS reloaded and enhanced with archival data  
 NEWS 32 MAY 21 TOXCENTER enhanced with BIOSIS reload  
 NEWS 33 MAY 21 CA/Caplus enhanced with additional kind codes for German patents  
 NEWS 34 MAY 22 CA/Caplus enhanced with IPC reclassification in Japanese patents  
 NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.  
 NEWS HOURS STN Operating Hours Plus Help Desk Availability  
 NEWS LOGIN Welcome Banner and News Items

NEWS IPCs For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 14:20:05 ON 29 MAY 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTARHH1626

PASSWORD:

\*\*\*\*\* RECONNECTED TO STN INTERNATIONAL \*\*\*\*\*

SESSION RESUMED IN FILE 'HOME' AT 14:27:19 ON 29 MAY 2007

FILE 'HOME' ENTERED AT 14:27:19 ON 29 MAY 2007

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.52	2.52

=&gt; file uspatall

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.52	2.52

FILE 'USPATFULL' ENTERED AT 14:27:25 ON 29 MAY 2007

CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATI' ENTERED AT 14:27:25 ON 29 MAY 2007

CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> # 4992204/pn  
 L1 0 4992204/PN

=> # 4992204/pa  
 L2 0 4992204/PA

=> # us4992204/pn  
 L3 1 US4992204/PN

=&gt; d ibib abs

L3 ANSWER 1 OF 1 USPATFULL on STN

ACCESSION NUMBER: 91:12712 USPATFULL Full-text  
 TITLE: Irradiation detection and identification method and compositions useful therein  
 INVENTOR(S): Kluger, Edward W., Pauline, SC, United States  
 Moore, Patrick D., Paeclet, SC, United States  
 Hines, John B., Spartanburg, SC, United States  
 Lever, John O., Spartanburg, SC, United States

PATENT ASSIGNEE(S): Miliken Research Corporation, Spartanburg, SC, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4992204		19910112
APPLICATION INFO.:	US 1989-397079		19890822 (7)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Niebling, John F.		
ASSISTANT EXAMINER:	Marquis, Steven P.		
LEGAL REPRESENTATIVE:	Monehan, Timothy J., Petry, H. William		
NUMBER OF CLAIMS:	35		
EXEMPLARY CLAIM:	1		
LINE COUNT:	2506		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A method for tagging one or a mixture of natural or synthetic materials comprising contacting the same with one or a mixture of tagging compounds containing one or more non-ionic luminophore moieties attached to at least one poly(oxyalkylene) moiety by means of a linking moiety; wherein said tagging compound has substantial absorbance within the range of from about 300 to about 400 nm and reemits substantial visible light, said contacting effecting at least a temporary association between said material and said compound wherein said compound is present in an amount between about 0.0001 and about 10 percent by weight of said material.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.94	7.46

FILE 'REGISTRY' ENTERED AT 14:28:06 ON 29 MAY 2007  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2  
 DICTIONARY FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

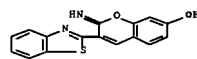
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> tra 13 rn  
 L4 TRANSFER L3 1- RN : 74 TERMS  
 L5 74 L4

=&gt; d scan

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 2H-1-Benzopyran-7-ol, 3-(2-benzothiazolyl)-2-imino- (9CI)  
 MF C16 H10 N2 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1,3-Isobenzofurandione, 4-nitro-  
 MF C8 H4 N O5  
 CI COM

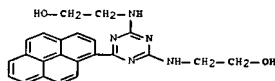


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with [[6-(1-pyrenyl)-1,3,5-triazine-2,4-diyl]diimino]bis[propanol] (2:1), dimethyl ether, block (9CI)  
 MF C25 H25 N5 O2 . 2 (C3 H6 O . C2 H4 O)x . 2 C H4 O

CM 1



2 (D1-Me)



CM 2

 $\text{H}_3\text{C}-\text{OH}$ 

CM 3

CM 4



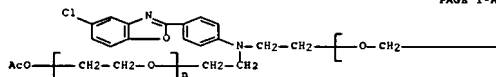
CM 5



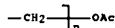
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Poly(oxy-1,2-ethanediyl),  $\alpha,\alpha'$ -[[[4-(5-chloro-2-benzoxazolyl)phenyl]imino]di-2,1-ethanediyl]bis[m-(acetyloxy)- (9CI)  
MF (C2 H4 O)n (C2 H4 O)n C21 H21 C1 N2 O5  
CI PMS

PAGE 1-A



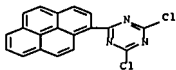
PAGE 1-B



CM 5



L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 1,3,5-Triazine, 2,4-dichloro-6-(1-pyrenyl)-  
MF C19 H9 Cl2 N3

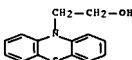


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Oxirane, methyl-, polymer with oxirane, 2-[[[4-(dimethylethyl)ethoxy] ether, block (9CI)  
MF C14 H13 N O 8 . (C3 H6 O . C2 H4 O)x . C H4 O

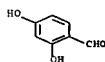
CM 1



CM 2

CM 3

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Benzaldehyde, 2,4-dihydroxy-  
MF C7 H6 O3  
CI COM

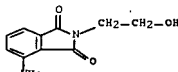


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Oxirane, methyl-, polymer with oxirane, 2-(4-amino-1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methylethyl methyl ether, block (9CI)  
MF C11 H12 N2 O3 . (C3 H6 O . C2 H4 O)x . C H4 O

CM 1



D1-Me

CM 2

 $\text{H}_3\text{C}-\text{OH}$ 

CM 3

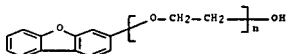
CM 4



CM 4



L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Poly(oxy-1,2-ethanediyl),  $\alpha$ -3-dibenzofuranyl-m-hydroxy- (9CI)  
MF (C2 H4 O)n C12 H8 O2  
CI PMS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

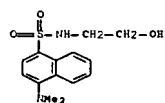
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Phenol, 2-amino-4-methyl-  
MF C7 H9 N O  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Oxirane, methyl-, polymer with oxirane, 2-[[[4-(dimethylethyl)ethoxy] ether, block (9CI)  
MF C15 H20 N2 O3 S . (C3 H6 O . C2 H4 O)x . C H4 O

CM 1



D1-Me

CM 2

H<sub>3</sub>C-OH

CM 3

CM 4

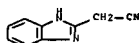


CM 5



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1H-Benzimidazole-2-acetonitrile  
 MF C9 H7 N3  
 CI COM

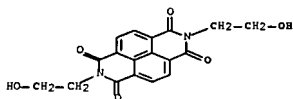


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with 2,7-bis(2-hydroxymethyl)ethylbenzo[1,2,3-cd]phenanthroline-1,3,6,8(2H,7H)-tetrone (2:1), dimethyl ether, block (9CI)  
 MF C20 H18 N2 O6 . 2 (C3 H6 O . C2 H4 O)x . 2 C H4 O

CM 1



2 ( D1-Me )

CM 2

H<sub>3</sub>C-OH

CM 3

CM 4

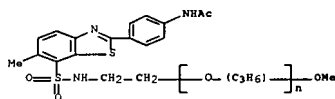


CM 5



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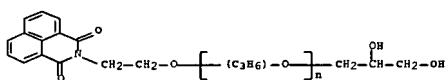
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-[2-[[[2-[4-(acetylamino)phenyl]-6-methyl-7-benzothiazolyl]sulfonyl]amino]methylethyl]-o-methoxy-(9CI)  
 MF (C3 H6 O)n C20 H23 N3 O4 S2  
 CI IDS, PMS



D1-Me

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-[2,3-dihydroxypropyl]-o-[2-(1,3-dioxo-1H-benz[de]isoquinolin-2(3H)-yl)methylethoxy]- (9CI)  
 MF (C3 H6 O)n C18 H19 N O5  
 CI IDS, PMS

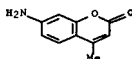


D1-Me

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Morpholine  
 MF C4 H9 N O  
 CI COM, RPS



L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 2H-1-Benzopyran-2-one, 7-amino-4-methyl-  
 MF C10 H9 N O2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

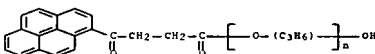
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1H,3H-Naphtho[1,8-cd]pyran-1,3-dione  
 MF C12 H6 O3  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-[1,4-dioxo-4-(1-pyrenyl)butyl]-o-hydroxy- (9CI)  
 MF (C3 H6 O)n C20 H14 O3  
 CI IDS, PMS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

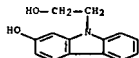
10/511852 13/217 Robert Havlin  
IN Benzenethiol, 2-amino-  
MF C6 H7 N S  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Oxirane, methyl-, polymer with oxirane, ether with 2-hydroxy-9H-carbazole-  
9-ethanol (2:1), block (9CI)  
MF C14 H13 N O2 . 2 (C3 H6 O . C2 H4 O)x

CM 1



CM 2

CM 3



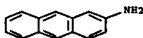
CM 4



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 1,3,5-Triazin-2-amine, 4,6-dichloro-N-[(4-(6-methyl-2-  
benzothiazolyl)phenyl)- (9CI)  
MF C17 H11 Cl2 N5 S

10/511852 15/217 Robert Havlin

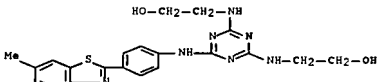


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Oxirane, methyl-, polymer with oxirane, ether with [[6-[[4-(6-methyl-2-  
benzothiazolyl)phenyl]amino]-1,3,5-triazine-2,4-diyl]diimino]bis[propanol]  
(2:1), dimethyl ether, block (9CI)  
MF C23 H27 N7 O2 S . 2 (C3 H6 O . C2 H4 O)x . 2 C H4 O

CM 1



2 (D1-Me)

CM 2

H3C-OH

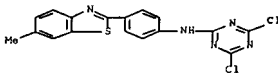
CM 3

CM 4



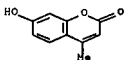
CM 5

10/511852 14/217 Robert Havlin



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

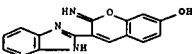
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-  
MF C10 H8 O3  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2H-1-Benzopyran-7-ol, 3-(1H-benzimidazol-2-yl)-2-imino- (9CI)  
MF C16 H11 N3 O2  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

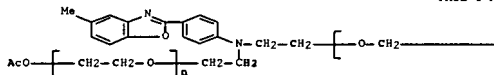
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2-Anthracenamine  
MF C14 H11 N  
CI COM

10/511852 16/217 Robert Havlin

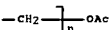


L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Poly(oxy-1,2-ethanediyl),  $\alpha,\alpha'$ -[[[4-(5-methyl-2-  
benzoxazolyl)phenyl]imino]di-2,1-ethanediyl]bis[m-(acetyloxy)- (9CI)  
MF (C2 H4 O)n (C2 H4 O)n C22 H24 N2 O5  
CI PMS

PAGE 1-A

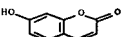


PAGE 1-B



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 2H-1-Benzopyran-2-one, 7-hydroxy-  
MF C9 H6 O3  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Oxirane, methyl-, polymer with oxirane, mono(2-oxo-2H-1-benzopyran-4-yl)  
ether (9CI)  
MF C9 H6 O3 . (C3 H6 O . C2 H4 O)x

CM 1



CM 2

CM 3

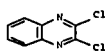


CM 4



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Quinoxaline, 2,3-dichloro-  
 MF C8 H4 Cl2 N2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, 2-[[[4-[[[3-hydroxy-2-naphthalenyl]carbonyl]amino]phenyl]sulfonyl]amino]methyl ethyl methyl ether, block (9CI)  
 MF C20 H20 N2 O5 S . (C3 H6 O . C2 H4 O)x . C H4 O  
 CM 1

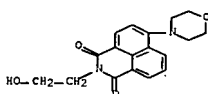
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Phenol, 2-amino-  
 MF C6 H7 N O  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, 2-[6-(4-morpholinyl)-1,3-dioxo-1H-benz[de]isoquinolin-2(3H)-yl]methyl ethyl methyl ether, block (9CI)  
 MF C19 H20 N2 O4 . (C3 H6 O . C2 H4 O)x . C H4 O  
 CM 1



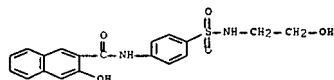
D1-Me

CM 2

H3C-OH

CM 3

CM 4



D1-Me

CM 2

H3C-OH

CM 3

CM 4

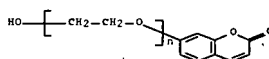


CM 5



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

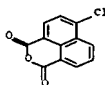
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy-1,2-ethanediyl], α-(2-oxo-2H-1-benzopyran-7-yl)-o-hydroxy- (9CI)  
 MF (C2 H4 O)n C9 H6 O3  
 CI PMS



CM 5



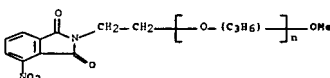
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1H,3H-Naphtho[1,8-cd]pyran-1,3-dione, 6-chloro-  
 MF C12 H5 Cl O3  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

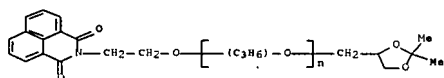
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-[2-(1,3-dihydro-4-nitro-1,3-dioxo-2H-isoindol-2-yl)methylethyl]-o-methoxy- (9CI)  
 MF (C3 H6 O)n C12 H12 N2 O5  
 CI IDS, PMS



D1-Me

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-[(2,2-dimethyl-1,3-dioxolan-4-yl)methyl]-o-[2-(1,3-dioxo-1H-benz[de]isoquinolin-2(3H)-yl)methylethoxy]- (9CI)  
 MF (C3 H6 O)n C21 H23 N O5  
 CI IDS, PMS



D1-Me

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

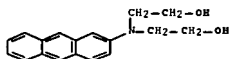
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1,3,5-Triazine, 2,4,6-trichloro-  
 MF C3 Cl3 N3  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with 2,2'-(2-anthracenylamino)bis[ethanol] (2:1), block (9CI)  
 MF C18 H15 N O2 . 2 (C3 H6 O . C2 H4 O)x  
 CI COM

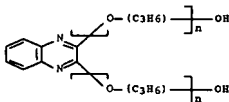
CM 1



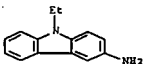
CM 2

CM 3

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)],  $\alpha,\alpha'$ -2,3-quinoxalinediylbis[ $\alpha$ -hydroxy- (9CI)  
 MF (C3 H6 O)n (C3 H6 O)n C8 H6 N2 O2  
 CI IDS, PMS



L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 9H-Carbazol-3-amine, 9-ethyl-  
 MF C14 H14 N2  
 CI COM

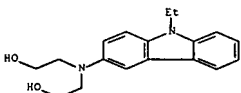


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with 2,2'-[(9-ethyl-9H-carbazol-3-yl)imino]bis[ethanol] (2:1), block (9CI)  
 MF C18 H22 N2 O2 . 2 (C3 H6 O . C2 H4 O)x  
 CI COM

CM 1

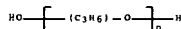


CM 4



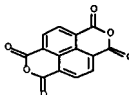
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)],  $\alpha$ -hydro- $m$ -hydroxy-  
 ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT  
 MF (C3 H6 O)n H2 O  
 CI IDS, PMS, COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN [2]Benzopyrano[6,5,4-def][2]benzopyran-1,3,6,8-tetrone  
 MF C14 H4 O6  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

CM 2

CM 3

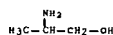


CM 4



L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, 2-methyl-, polymer with oxirane, 2-aminopropyl methyl ether  
 MF C3 H9 N O . (C3 H6 O . C2 H4 O)x . C H4 O  
 CI COM

CM 1



CM 2

H3C-OH

CM 3

CM 4



CM 5

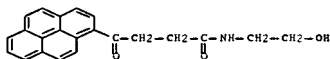




HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, 2-[[1,4-dioxo-4-(1-pyrenyl)butyl]amino]methyl ether, block (9CI)  
 MF C23 H21 N O3 . (C3 H6 O . C2 H4 O)x . C H4 O

CM 1



D1-Me

CM 2

H3C-OH

CM 3

CM 4



CM 5



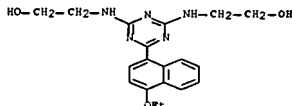
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1,3,5-Triazine, 2,4-dichloro-6-(4-ethoxy-1-naphthalenyl)- (9CI)  
 MF C15 H11 Cl2 N3 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with [[6-(4-ethoxy-1-naphthalenyl)-1,3,5-triazine-2,4-diyl]diimino]bis[propanol] (2:1), dimethyl ether, block (9CI)  
 MF C21 H27 N5 O3 . 2 (C3 H6 O . C2 H4 O)x . 2 C H4 O

CM 1



2 ( D1-Me )

CM 2

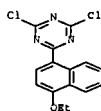
H3C-OH

CM 3

CM 4



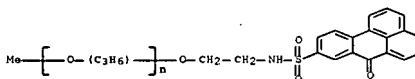
CM 5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

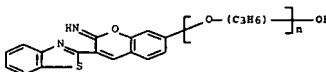
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-methyl-ω-[methyl-1-[[[7-oxo-7H-benz[de]anthracen-9-yl]sulfonyl]amino]epoxy]- (9CI)  
 MF (C3 H6 O)n C21 H19 N O4 S  
 CI IDS, PMS



D1-Me

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-methyl-ω-[methyl-1-[[[7-oxo-7H-benz[de]anthracen-9-yl]sulfonyl]amino]epoxy]- (9CI)  
 MF (C3 H6 O)n C16 H10 N2 O2 S  
 CI IDS, PMS



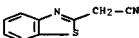
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Pyrene  
 MF C16 H10  
 CI COM, RPS



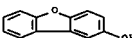
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 2-Benzothiazoleacetonitrile  
 MF C9 H6 N2 S  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

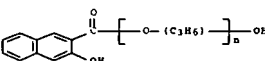
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 2-Dibenzofuranol  
 MF C12 H8 O2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly[oxy(methyl-1,2-ethanediyl)], α-[[3-hydroxy-2-naphthalenyl]carbonyl]-ω-hydroxy- (9CI)  
 MF (C3 H6 O)n C11 H8 O3  
 CI IDS, PMS





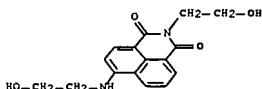
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 1-Naphthalenesulfonyl chloride, 5-(dimethylamino)-  
 MF C13 H12 Cl N O2 S  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with 2-(2-hydroxymethylethyl)-6-[[[2-hydroxymethylethyl]amino]-1H-benz[de]isoquinoline-1,3(2H)-dione (2:1), dimethyl ether, block (9CI)  
 MF C18 H20 N2 O4 . 2 (C3 H6 O . C2 H4 O)x . 2 C H4 O  
 CM 1



2 (DI-Me)

CM 2

H3C-OH

CM 3

CM 4

ALL ANSWERS HAVE BEEN SCANNED

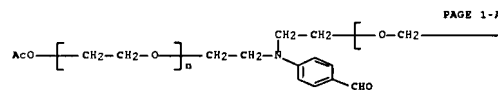
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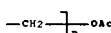
CM 5



L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Poly(oxy-1,2-ethanediyl), α,α'-[[[4-formylphenyl]imino]di-2,1-ethanediyl]bis[α-(acetyloxy)- (9CI)  
 MF C2 H4 O)n (C2 H4 O)n C15 H19 N O5  
 CI PMS



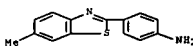
PAGE 1-A



PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

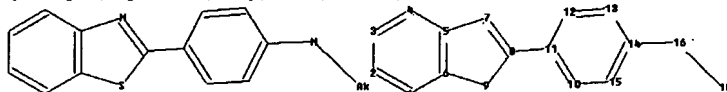
L5 74 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-  
 MF C14 H12 N2 S  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

>>

Uploading C:\Program Files\Stnexp\Queries\10.511852\clm16.str



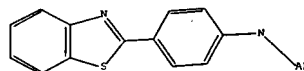
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 16 18  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15  
 chain bonds :  
 8-11 14-16 16-18  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15  
 exact/norm bonds :  
 5-7 7-8 14-16 16-18  
 exact bonds :  
 6-9 8-9 8-11  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15  
 isolated ring systems :  
 containing 1 : 10 :

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS  
 Element Count :  
 Node 18: Limited  
 C,C,S

L6 STRUCTURE UPLOADED

>> d

L6 HAS NO ANSWERS  
 L6 STR



Structure attributes must be viewed using STN Express query preparation.

>> a 16 sss sam  
 SAMPLE SEARCH INITIATED 14:30:56 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 546 TO ITERATE

100.0% PROCESSED 546 ITERATIONS 4 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 9519 TO 12321  
 PROJECTED ANSWERS: 4 TO 200

L7 4 SEA SSS SAM L6

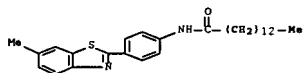
>> a 16 sss full  
 FULL SEARCH INITIATED 14:31:02 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 10584 TO ITERATE

100.0% PROCESSED 10584 ITERATIONS 127 ANSWERS  
 SEARCH TIME: 00.00.01

L8 127 SEA SSS FUL L6

>> d scan

L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Tetradecanamide, N-[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI)  
 MF C28 H38 N2 O S

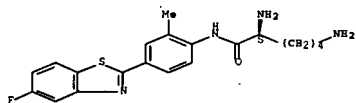


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

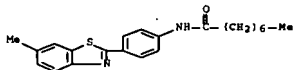
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, (2S)- (9CI)  
 MF C20 H23 F N4 O S  
 CI COM

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

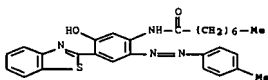
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Octanamide, N-[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI)  
 MF C22 H26 N2 O S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

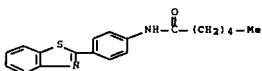
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(4-methylphenyl)azo]phenyl]- (9CI)  
 MF C28 H30 N4 O3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

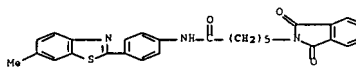
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Hexanamide, N-[4-(2-benzothiazolyl)phenyl]-  
 MF C19 H20 N2 O S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

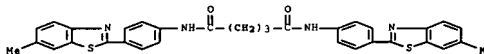
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 2H-Isaondole-2-hexanamide, 1,3-dihydro-N-[4-(6-methyl-2-benzothiazolyl)phenyl]-1,3-dioxo- (9CI)  
 MF C28 H25 N3 O3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

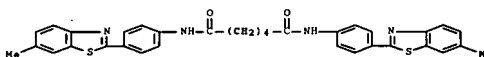
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Pentanediamide, N,N'-bis[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI)  
 MF C33 H28 N4 O2 S2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Hexanediamide, N,N'-bis[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI)  
 MF C34 H30 N4 O2 S2

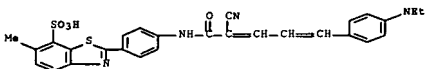


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

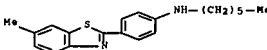
L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl- (8CI)  
 MF C30 H28 N4 O4 S2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8 127 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Benzenamine, N-hexyl-4-(6-methyl-2-benzothiazolyl)- (9CI)  
 MF C20 H24 N2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

>> d hist

(FILE 'HOME' ENTERED AT 14:20:05 ON 29 MAY 2007)

FILE 'USPATFULL, USPAT2' ENTERED AT 14:27:25 ON 29 MAY 2007  
 L1 0 S 4992204/PN  
 L2 0 S 4992204/PN  
 L3 1 S US4992204/PN

FILE 'REGISTRY' ENTERED AT 14:28:06 ON 29 MAY 2007

FILE 'USPATFULL' ENTERED AT 14:28:12 ON 29 MAY 2007  
 TRA L3 1- RN : 74 TERMS

FILE 'REGISTRY' ENTERED AT 14:28:13 ON 29 MAY 2007  
 L5 74 SEA L4

STRUCTURE UPLOADED  
L6 4 S L6 SSS SAM  
L7 127 S L6 SSS FULL  
L8

== file hcaplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL ENTRY	SESSION
174.35	194.93	

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 14:31:44 ON 29 MAY 2007  
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FILE COVERS 1907 - 29 May 2007 VOL 146 ISS 23  
FILE LAST UPDATED: 28 May 2007 (20070528/BD)

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== s 18  
L9 24 L8

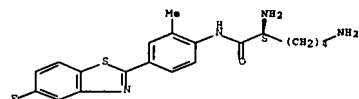
== d ibib abs hitstr tot

L9 ANSWER 1 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2006:1210169 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 146:155514  
TITLE: In vitro cytotoxicity of Phortress against colorectal cancer  
AUTHOR(S): Mukherjee, Abhik; Graham Martin, Stewart  
CORPORATE SOURCE: Department of Oncology, City Hospital, University of Nottingham, Nottingham, NG5 1PB, UK  
SOURCE: International Journal of Oncology (2006), 29(5), 1287-1294  
CODEN: IJONES; ISSN: 1019-6439  
PUBLISHER: International Journal of Oncology  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Phortress is a novel benzothiazole compound with activity concentrated in certain breast, ovarian and renal cancer cell lines. Its anti-angiogenic effects are unknown. In this study, the in vitro anti-angiogenic effects of Phortress were screened for and results compared with two control drugs, paclitaxel and fumagillin. In vitro anti-angiogenic activity was examined by MTS assays, growth curves and clonogenic survival assays on human umbilical vein endothelial cells (HUEVC). In addition and as a comparator, effects were examined on MRCV fibroblasts and also the MCF7 breast cancer cell line, shown to be sensitive on the NCI60 panel and 3 colorectal cancer cell lines (HT29, SW480 and SW620) that were reportedly insensitive. Effects on endothelial tube differentiation were assessed by the Matrigel assay. Phortress had no effect on HUEVC and MRCV cell proliferation and survival. Unlike paclitaxel and fumagillin, Phortress did not inhibit

used in patient with cancer)  
RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCL

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:6103 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 142:385200  
TITLE: In vitro, in vivo, and in silico analyses of the antitumor activity of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazoles  
AUTHOR(S): Leong, Chee Onn; Suggitt, Marie; Swaine, David J.; Bibby, Michael C.; Stevens, Malcolm F. G.; Bradshaw, Tracey D.  
CORPORATE SOURCE: Centre for Biomolecular Sciences, School of Pharmacy, University of Nottingham, Nottingham, UK  
SOURCE: Molecular Cancer Therapeutics (2004), 3(12), 1565-1575  
CODEN: MCTGCF; ISSN: 1535-7163  
PUBLISHER: American Association for Cancer Research  
DOCUMENT TYPE: Journal  
LANGUAGE: English

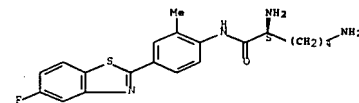
AB Phortress is a novel, potent, and selective exptl. antitumor agent. Its mechanism of action involves induction of CYP1A1-catalyzed biotransformation of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole (5F 203) to generate electrophilic species, which covalently bind to DNA, exacting lethal damage to sensitive tumor cells, in vitro and in vivo. Herein, we investigate the effects of DNA adduct formation on cellular DNA integrity and progression through cell cycle and examine whether a relevant pharmacodynamic end point may be exploited to probe the clin. mechanism of action of Phortress and predict tumor response. Single cell gel electrophoresis (SCGE) was applied to quantify DNA damage and cell cycle analyses conducted upon 5F 203 treatment of benzothiazole-sensitive MCF-7 and inherently resistant MDA-MB-435 breast carcinoma cells. Following treatment of xenograft-bearing mice and mice possessing hollow fiber implants containing MCF-7 or MDA-MB-435 cells with Phortress (20 mg/kg, i.p., 24 h), tumor cells and xenografts were recovered for analysis by SCGE. Dose- and time-dependent DNA single and double strand breaks occurred exclusively in sensitive cells following treatment with 5F 203 in vitro (10 nmol/L-10 μmol/L; 24-72 h). In vivo, Phortress-sensitive and Phortress-resistant tumor cells were distinct; moreover, DNA damage in xenografts, following treatment of mice with Phortress, could be determined. Interrogation of the mechanism of action of 5F 203 in silico by self-organizing map-based cluster analyses revealed modulation of phosphatases and kinases associated with cell cycle regulation, corroborating observations of selective cell cycle perturbation by 5F 203 in sensitive cells. By conducting SCGE, tumor sensitivity to Phortress, an agent currently undergoing clin. evaluation, may be determined

IT 328087-38-3, Phortress

endothelial tube differentiation. Phortress therefore exhibits no in vitro anti-angiogenic activity. As expected, Phortress was cytotoxic to MCF7 breast cancer cells, but unexpectedly, Phortress was also potent against colorectal cancer cells in clonogenic survival and cell growth (growth curves but not MTS assay) end-points. The efficacy of Phortress against colorectal cancer cells in the current study confirms that the spectrum of activity of Phortress may be wider than previously thought.

IT 328087-38-3, Phortress  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(anti-angiogenic and cytotoxic activity of Phortress against breast and colorectal cancer cells)  
RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCL

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:1097867 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 144:141573  
TITLE: Update to: The Aryl Hydrocarbon Receptor in Anticancer Drug Discovery: Friend or foe?  
AUTHOR(S): Bradshaw, T. D.; Mortimer, C. G.; Westwell, A. D.  
CORPORATE SOURCE: Centre for Biomolecular Sciences, School of Pharmacy, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Medicinal Chemistry Reviews--Online (2005), 2(2), 153-161  
CODEN: MCREC9; ISSN: 1567-2034  
URL: <http://www.ingentaconnect.com/content/ben/mcro/2005/00000002/00000002>  
PUBLISHER: Bentham Science Publishers Ltd.  
DOCUMENT TYPE: Journal; General Review; (online computer file)  
LANGUAGE: English

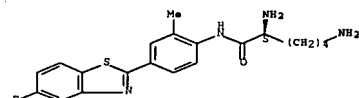
AB A review. Major advances in our understanding of the mechanistic features and regulation of Aryl hydrocarbon Receptor (Ahr) mediated signal transduction have been made in recent years. This review updates our previously published article "The Aryl Hydrocarbon Receptor in Anticancer Drug Discovery: Friend or foe", focussing on the most recent developments in the field. Discussion of receptor regulation and crosstalk, structural studies on the ligand binding domain, the search for endogenous ligands, and therapeutic possibilities in the cancer field associated with Ahr ligands, feature prominently here.

IT 328087-38-3, Phortress  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(aryl hydrocarbon receptor agonist, 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole, active component of prodrug Phortress binding induced CYP1A1 which converted it to cytotoxic intermediate thus can be

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(in vitro, in vivo, and in silico analyses of antitumor activity of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazoles)

RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCL

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:757951 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 142:348246  
TITLE: The Experimental Antitumor Agents Phortress and Doxorubicin are Equiactive Against Human-Derived Breast Carcinoma Xenograft Models  
AUTHOR(S): Fichtner, Iduna; Monks, Anne; Hesse, Curtis; Stevens, Malcolm F. G.; Bradshaw, Tracey D.  
CORPORATE SOURCE: Max-Delbrueck Center for Molecular Medicine, Experimental Pharmacology, Berlin, Germany  
SOURCE: Breast Cancer Research and Treatment (2004), 87(1), 97-107  
CODEN: BCTRDE; ISSN: 0167-6806  
PUBLISHER: Kluwer Academic Publishers  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Phortress (the dihydrochloride salt of the lysylamide prodrug of 2-(4-amino-3-methylphenyl)-5-fluoro-benzothiazole (5F 203)) is an exptl. antitumor agent with potent and selective activity against human-derived carcinomas of breast, ovarian and renal origin. The mechanism of action of Phortress is distinct from all classes of chemotherapeutic agents currently in the clinic, and involves metabolic activation by cytochrome P 450 (CYP) 1A1 to electrophilic species, which generate DNA adducts in sensitive tumors only. In the present study, the antitumor efficacy of Phortress has been compared with that of doxorubicin (Dox) in nine human-derived mammary carcinoma xenograft models, cultivated s.c. in the flanks of nude mice. In addition, cyp1a1 mRNA expression was measured in tumors of control and treated animals. Phortress compared favorably with Dox: significant activity, independent of estrogen receptor (ER) status, was established in 7/9 xenografts; in one xenograft model, Phortress elicited superior antitumor activity; no model demonstrated complete resistance to Phortress. In accordance with this observation, all xenografts available for examination (8) displayed clear induction of cyp1a1 expression upon treatment of mice with Phortress whereas Dox failed to induce cyp1a1 expression in all models. Prolonged viability of tumor fragments, recovered for treatment ex vivo could not be sustained; thus correlations between tumor cells' response to Phortress and cyp1a1 or cyp1b1 inducibility following 5F 203 treatment could not be determined with confidence.

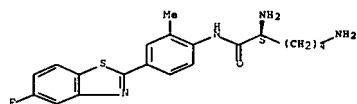
IT 328087-38-3, NSC 710305

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Phoresis; exptl; anticancer agents Phortress and doxorubicin are equiactive against human-derived breast carcinoma xenograft models)

RN 328087-38-3 HCAPLUS

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RR FORMAT

L9 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 2004:633552 HCAPLUS Full-text  
DOCUMENT NUMBER: 141:179563  
TITLE: Amyloid-binding, metal-chelating imaging and therapeutic agents  
INVENTOR(S): Huang, Xudong  
PATENT ASSIGNEE(S): The General Hospital Corporation, USA  
SOURCE: PCT Int. Appl., 99 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004064869	A2	20040805	WO 2004-US1669	20040122
WO 2004064869	A3	20050324		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GR, GM, GU, HU, ID, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NZ, OM, OS, PA, PE, PG, PH, PI, PT, RO, RU, SC, SE, SG, SI, SK, SL, SM, SN, ST, SV, SZ, TD, TH, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
AU 2004206956	A1	20040805	AU 2004-206956	20040122
CA 2514200	A1	20040805	CA 2004-2514200	20040122
EP 1587547	A2	20051026	EP 2004-704402	20040122
R: AT, BR, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1774267	A	20060517	CN 2004-80004902	20040122
JP 2006515630	T	20060601	JP 2006-501093	20040122
IN 2005KN1662	A	20060922	IN 2005-KN1662	20050819
PRIORITY APPLN. INFO.:			US 2003-441719P	P 20030122
			WO 2004-US1669	W 20040122

OTHER SOURCE(S): MARPAT 141:179563

AB The present invention relates to the diagnosis, prevention, and treatment of pathophysiological conditions associated with amyloid accumulation. Bifunctional therapeutic moles. and contrast imaging agents exhibiting a high affinity for amyloid deposits, and

pharmaceutical compns. thereof are described. The invention also provides methods of using these bifunctional moles., contrast imaging agents, and pharmaceutical compns. for detecting the presence of amyloid deposits using imaging techniques; and for preventing or treating amyloid-related conditions, such as, for example, Alzheimer's disease.

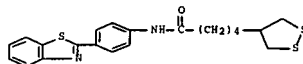
IT 731809-56-5D, conjugated complexes

RL: DGN (Diagnostic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(amyloid-binding, metal-chelating imaging and therapeutic agents)

RN 731809-56-6 HCAPLUS

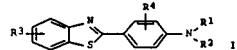
CN 1,2-Dithiolane-4-pentanamide, N-[4-(2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)



L9 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 2003:836808 HCAPLUS Full-text  
DOCUMENT NUMBER: 139:327931  
TITLE: Aminophenyl-benzothiazole compounds as UV filters in cosmetics  
INVENTOR(S): Wagner, Barbara; Ehlig, Thomas; Mongiat, Sebastien; Eichin, Kai  
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.  
SOURCE: PCT Int. Appl., 48 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003086341	A2	20031023	WO 2003-EP3870	20030414
WO 2003086341	A3	20040401		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GR, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NZ, OM, OS, PA, PE, PG, PH, PI, PT, RO, RU, SC, SE, SG, SI, SK, SL, SM, SN, ST, SV, SZ, TD, TH, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RU 2003229665	A1	20031027	AU 2003-229665	20030414
EP 1494641	A2	20050112	EP 2003-722472	20030414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 200309308	A	20050215	BR 2003-9308	20030414
CN 1646507	A	20050727	CN 2003-808638	20030414
US 2005175554	A1	20050811	US 2003-511852	20030414
JP 200529869	T	20051006	JP 2003-583365	20030414
IN 2004CN02585	A	20070302	IN 2004-CN2585	20041117
PRIORITY APPLN. INFO.:			EP 2002-405311	A 20020417
			CH 2002-2135	A 20021216

OTHER SOURCE(S): MARPAT 139:327931  
OI



AB The preparation and use, as a UV filter, of a compound of formula I (R1, R2 = H, unsubstituted or halo-, amino-, mono- or di-C1-5-alkylamino-, cyano- or C1-5-alkoxy-substituted C1-22-alkyl, C5-10-cycloalkyl, carboxy-C1-22-alkyl, carboxy-C6-10-aryl, C6-10-aryl, C6-10-aryl-C1-5-alkyl; carbamoyl; sulfamoyl; R1, R2, N forming 5- to 7-membered heterocyclic radical; R3 = H, C1-22-alkyl; R4 = H, OH, C1-22-alkyl, C1-22-alkoxy) is described. The compds. of formula I in micronized form are suitable as UV absorbers in cosmetic preps. and for protecting hair and skin from UV radiation.

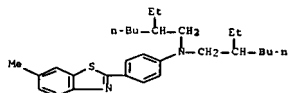
IT 614717-93-OP 614717-94-1P 614717-96-3P  
614717-97-4P 614717-99-6P 614718-00-2P  
614718-02-4P 614718-04-6P 614718-05-7P  
614718-09-0P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and cosmetic use of aminophenyl benzothiazole compds. as UV filters)

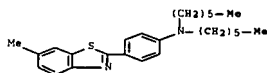
RN 614717-93-0 HCAPLUS

CN Benzenamine, N,N-bis(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



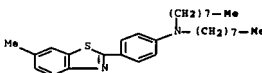
RN 614717-94-1 HCAPLUS

CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



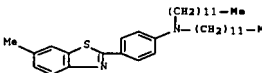
RN 614717-96-3 HCAPLUS

CN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-N,N-dioctyl- (9CI) (CA INDEX NAME)



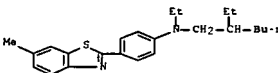
RN 614717-97-4 HCAPLUS

CN Benzenamine, N,N-didodecyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



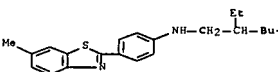
RN 614717-99-6 HCAPLUS

CN Benzenamine, N-ethyl-N-(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



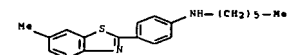
RN 614718-00-2 HCAPLUS

CN Benzenamine, N-(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)

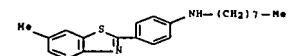


RN 614718-02-4 HCAPLUS

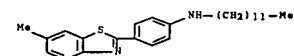
CN Benzenamine, N-hexyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



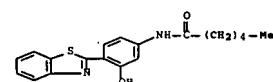
RN 614718-04-6 HCAPLUS  
CN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-N-octyl-, (9CI) (CA INDEX NAME)



RN 614718-05-7 HCAPLUS  
CN Benzenamine, N-dodecyl-4-(6-methyl-2-benzothiazolyl)-, (9CI) (CA INDEX NAME)



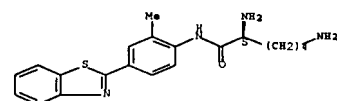
RN 614718-08-0 HCAPLUS  
CN Hexanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]-, (9CI) (CA INDEX NAME)



L9 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:356035 HCAPLUS Full-text  
DOCUMENT NUMBER: 138:355189  
TITLE: Dyes with counterions for reduction of inkjet decap and for improvement of durability of images  
INVENTOR(S): Schut, David M.; Schmid, Christian  
PATENT ASSIGNEE(S): Hewlett-Packard Company, USA  
SOURCE: Eur. Pat. Appl., 36 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

RN 328087-34-9 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)-, (2S)- (9CI) (CA INDEX NAME)

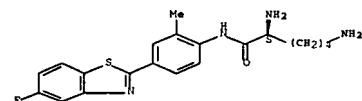
Absolute stereochemistry.



● 2 HC1

RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (1:2), (2S)- (9CI) (CA INDEX NAME)

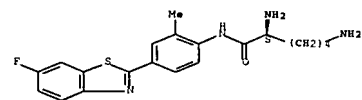
Absolute stereochemistry.



● 2 HC1

RN 328087-39-4 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

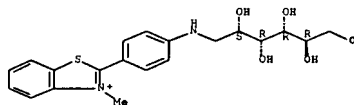
Absolute stereochemistry.



● 2 HC1

PATENT NO. KIND DATE APPLICATION NO. DATE  
EP 1308482 A1 20030507 EP 2002-257314 20021022  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IS, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK  
US 2003127017 A1 20030710 US 2001-4148 20011031  
US 7094277 B2 20060822  
JP 2003201415 A 20030718 JP 2002-318161 20021031  
PRIORITY APPLN. INFO.: US 2001-4148 A 20011031  
OTHER SOURCE(S): MARPAT 138:355189  
AB Dyes for ink-jet printing on both hydrophilic and hydrophobic papers are disclosed. The dyes include a chromophore ionically coupled to a counterion. One of the chromophore and the counterion includes a hydrophilic moiety. The other includes a hydrophobic moiety. Examples of ionic dyes, especially azo dyes, were given.  
IT 521086-59-9  
RL: TEM (Technical or engineered material use); USES (Uses)  
(ionic dyes with counterions for improved jet printing ink performance)  
RN 521086-59-9 HCAPLUS  
CN D-Glucitol, 1-deoxy-1-[[4-(1-methylbenzothiazolium-2-yl)phenyl]amino]-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.



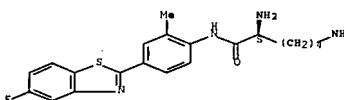
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:241156 HCAPLUS Full-text  
DOCUMENT NUMBER: 140:35389  
TITLE: Preclinical evaluation of amino acid prodrugs of novel antitumor 2-(4-amino-3-methylphenyl)benzothiazoles. [Erratum to document cited in CA137:72775]  
AUTHOR(S): Bradshaw, Tracey D.; Bibby, Michael C.; Double, John A.; Pichtner, Iduna; Cooper, Patricia A.; Alley, Michael C.; Donohue, Susan; Stinson, Sherman P.; Tomaszewski, Joseph E.; Sausville, Edward A.; Stevens, Malcolm F. O.  
CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Molecular Cancer Therapeutics (2003), 2(2), 207  
CODEN: MCTOCP; ISSN: 1535-7163  
PUBLISHER: American Association for Cancer Research  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB In Figure 3, panels B and C were transposed; the corrected figure is given.  
IT 328087-34-9 328087-38-3 328087-39-4  
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preclin. evaluation of amino acid prodrugs of antitumor

L9 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:87659 HCAPLUS Full-text  
DOCUMENT NUMBER: 139:316727  
TITLE: Antitumour 2-(4-aminophenyl)benzothiazoles generate DNA adducts in sensitive tumour cells in vitro and in vivo  
AUTHOR(S): Leong, C.-O.; Gaskell, M.; Martin, E. A.; Heydon, R. T.; Farmer, P. B.; Bibby, M. C.; Cooper, P. A.; Double, J. A.; Bradshaw, T. D.; Stevens, M. F. G.  
CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: British Journal of Cancer (2003), 88(3), 470-477  
CODEN: BJCAAI; ISSN: 0007-0920  
PUBLISHER: Nature Publishing Group  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB 2-(4-Aminophenyl)benzothiazoles represent a potent and highly selective class of antitumor agent. In vitro, sensitive carcinoma cells deplete 2-(4-aminophenyl)benzothiazoles from nutrient media; cytochrome P 450 1A1 activity, critical for execution of antitumor activity, and protein expression are powerfully induced. 2-(4-Amino-3-methylphenyl)benzothiazole-derived covalent binding to cytochrome P 450 1A1 is reduced by glutathione, suggesting 1A1-dependent production of a reactive electrophilic species. In vitro, 2-(4-aminophenyl)benzothiazole-generated DNA adducts form in sensitive tumor cells only. At concns. >100 nM, adducts were detected in DNA of MCF-7 cells treated with 2-(4-aminophenyl)-5-fluorobenzothiazole (5F 203). 5F 203 (1 μM) led to the formation of one major and a number of minor adducts. However, treatment of cells with 10 μM 5F 203 resulted in the emergence of a new dominant adduct. Adducts accumulated steadily within DNA of MCF-7 cells exposed to 1 μM 5F 203 between 2 and 24 h. Concns. of the lysylamide prodrug of 5F 203 (Phortress) 2100 nM generated adducts in the DNA of sensitive MCF-7 and IGROV-1 ovarian cells. At 1 μM, one major Phortress-derived DNA adduct was detected in these two sensitive phenotypes; 10 μM Phortress led to the emergence of an addnl. major adduct detected in the DNA of MCF-7 cells. Inherently resistant MDA-MB-435 breast carcinoma cells incurred no DNA damage upon exposure to Phortress (≤10 μM, 24 h). In vivo, DNA adducts accumulated within sensitive ovarian IGROV-1 and breast MCF-7 xenografts 24 h after treatment of mice with Phortress (20 mg kg<sup>-1</sup>). Moreover, Phortress-derived DNA adduct generation distinguished sensitive MCF-7 tumors from inherently resistant MDA-MB-435 xenografts implanted in opposite flanks of the same mouse.  
IT 328087-38-3, MSC 710305  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(antitumor 2-(4-aminophenyl)benzothiazoles generate DNA adducts in sensitive tumor cells in vitro and in vivo)  
RN 328087-38-3 HCAPLUS  
CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (1:2), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 HC1

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

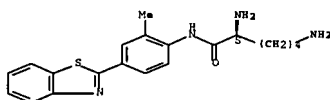
L9 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2002:440574 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 138:49377  
 TITLE: In vitro evaluation of amino acid prodrugs of novel antitumor 2-(4-amino-3-methylphenyl)benzothiazoles  
 Bradshaw, T. D.; Chua, M. S.; Browne, H. L.; Trapani, V.; Sausville, E. A.; Stevens, M. F. G.  
 CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
 SOURCE: British Journal of Cancer (2002), 86(8), 1348-1354  
 CODEN: BJCAAI; ISSN: 0007-0920  
 PUBLISHER: Nature Publishing Group  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Novel 2-(4-aminophenyl)benzothiazoles possess highly selective, potent antitumor properties in vitro and in vivo. They induce and are biotransformed by cytochrome P 450 (CYP) 1A1 to putative active as well as inactive metabolites. Metabolic inactivation of the mol. has been thwarted by isosteric replacement of hydrogen with fluorine atoms at positions around the benzothiazole nucleus. The lipophilicity of these comds. presents limitations for drug formulation and bioavailability. To overcome this problem, water soluble prodrugs have been synthesized by conjugation of alanyl- and lysyl-amide hydrochloride salts to the exocyclic primary amine function of 2-(4-aminophenyl)benzothiazoles. The prodrugs retain selectivity with significant in vitro growth inhibitory potency against the same sensitive cell lines as their parent amine, but are inactive against cell lines inherently resistant to 2-(4-aminophenyl)benzothiazoles. Alanyl and lysyl prodrugs rapidly and quant. revert to their parent amine in sensitive and insensitive cell lines in vitro. Liberated parent comds. are sequestered and metabolized by sensitive cells only; similarly, CYP1A1 activity and protein expression are selectively induced in sensitive carcinoma cells. Amino acid prodrugs meet the criteria of aqueous solubility, chemical stability and quant. reversion to parent mol., and thus are suitable for in vivo preclin. evaluation.

IT 328087-34-9 328087-38-3 328087-39-4  
 328087-50-9  
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USBS (Uses)  
 (in vitro evaluation of amino acid prodrugs of novel antitumor amino methylphenyl benzothiazoles)

RN 328087-34-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

RN 328087-38-3 HCAPLUS

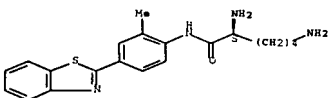
L9 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2002:230849 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 137:72775  
 TITLE: Preclinical evaluation of amino acid prodrugs of novel antitumor 2-(4-amino-3-methylphenyl)benzothiazoles  
 Bradshaw, Tracey D.; Bibby, Michael C.; Double, John A.; Pichtner, Iduna; Cooper, Patricia A.; Alley, Michael C.; Donohue, Susan; Stinson, Sherman F.; Tomaszewski, Joseph E.; Sausville, Edward A.; Stevens, Malcolm F. G.  
 CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
 SOURCE: Molecular Cancer Therapeutics (2002), 1(4), 239-246  
 CODEN: MCTOCP; ISSN: 1535-7163  
 PUBLISHER: American Association for Cancer Research  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Novel 2-(4-aminophenyl)benzothiazoles possess highly selective, potent antitumor properties in vitro and in vivo. Elucidation of the mechanism of action of this structurally simple class of comds. has occurred in parallel with selection of a candidate clin. agent. Antitumor benzothiazoles induce and are biotransformed by cytochrome P 450 1A1 to putative active, as well as inactive metabolites. Metabolic inactivation of the mol. has been thwarted by isosteric replacement of hydrogen with fluorine atoms at positions around the benzothiazole nucleus. Amino acid conjugation to the exocyclic primary amine function of 2-(4-aminophenyl)benzothiazoles has been used to overcome limitations posed by drug lipophilicity. Water soluble, chemical stable prodrugs rapidly and quant. revert to their parent amine in mice, rats, and dogs in vivo. Plasma concns. of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole regenerated from the lysylamide prodrug (I), sufficient to elicit cytotoxic activity against ZR-75-1 and T47D human mammary carcinoma cell lines persist > 6 h. The growth of breast (MCF-7) and ovarian (IGROV-1) xenograft tumors is significantly retarded by I. Manageable toxic side effects are reported from pre-clin. efficacious doses of I. Cytochrome P 450 1A1 protein expression, selectively induced in sensitive carcinoma cells, was detected in MCF-7 and IGROV-1 tumors 24 h after treatment of mice with I (20 mg/kg). The lysyl amide prodrug of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole is potentially suitable for clin. evaluation.

IT 328087-34-9 328087-38-3 328087-39-4  
 RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USBS (Uses)  
 (preclin. evaluation of amino acid prodrugs of antitumor 2-(4-amino-3-methylphenyl)benzothiazoles)

RN 328087-34-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

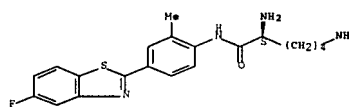
Absolute stereochemistry.



●2 HCl

CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

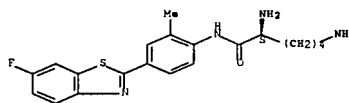
Absolute stereochemistry.



●2 HCl

RN 328087-39-4 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

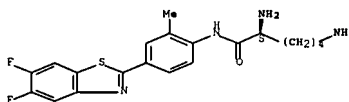
Absolute stereochemistry.



●2 HCl

RN 328087-50-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5,6-difluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

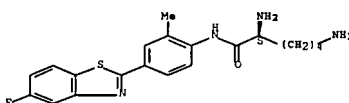


●2 HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RN 328087-38-3 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

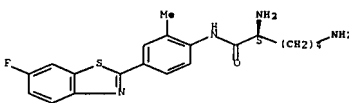
Absolute stereochemistry.



●2 HCl

RN 328087-39-4 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(6-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

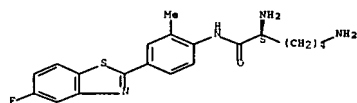
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2001:918063 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 136:184083  
 TITLE: Antitumor Benzothiazoles. 16. Synthesis and Pharmaceutical Properties of Antitumor 2-(4-Aminophenyl)benzothiazole Amino Acid Prodrugs  
 Hutchinson, Ian; Jennings, Sharon A.; Vishnuvajjala, B. Rao; Westwell, Andrew D.; Stevens, Malcolm F. G.  
 CORPORATE SOURCE: Cancer Research Laboratories School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
 SOURCE: Journal of Medicinal Chemistry (2002), 45(3), 744-747  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:184083

AB A series of water-soluble L-lysyl- and L-alanyl-amide prodrugs of the lipophilic antitumor 2-(4-aminophenyl)benzothiazoles has been synthesized to address formulation and bioavailability issues related to the desired parenteral administration of the chosen clin. candidate. The prodrugs exhibit the required pharmaceutical properties of good water solubility (in weak acid) and stability at ambient temperature and degradation to free base in vivo. The lysyl-amide of 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole (NSC 710305) has been selected for phase 1 clin. evaluation.

IT 328087-38-3P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (synthesis of antitumor (aminophenyl)benzothiazole amino acid prodrugs)  
 RN 328087-38-3 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

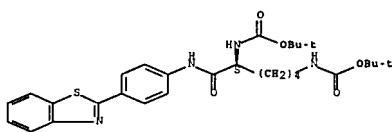
Absolute stereochemistry.



● 2 HCl

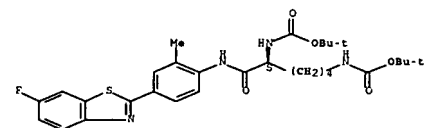
IT 398478-05-2P 398478-07-4P 398478-08-5P  
 398478-09-6P 398478-10-9P 398478-11-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis of antitumor (aminophenyl)benzothiazole amino acid prodrugs)  
 RN 398478-05-2 HCAPLUS  
 CN Carbamic acid, [(1S)-1-[[[4-(2-benzothiazolyl)phenyl]amino]carbonyl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



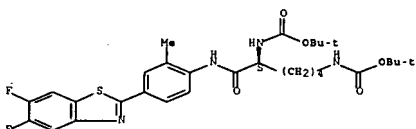
RN 398478-07-4 HCAPLUS  
 CN Carbamic acid, [(1S)-1-[[[4-(2-benzothiazolyl)-2-methylphenyl]amino]carbonyl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



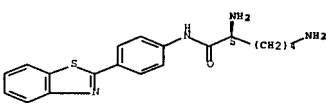
RN 398478-11-0 HCAPLUS  
 CN Carbamic acid, [(1S)-1-[[[4-(5,6-difluoro-2-benzothiazolyl)-2-methylphenyl]amino]carbonyl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 328087-33-8P 328087-34-9P 328087-35-0P  
 328087-39-4P 328087-50-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of antitumor (aminophenyl)benzothiazole amino acid prodrugs)  
 RN 328087-33-8 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)phenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

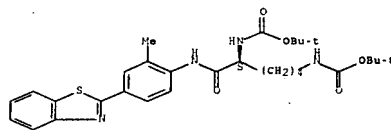
Absolute stereochemistry.



● 2 HCl

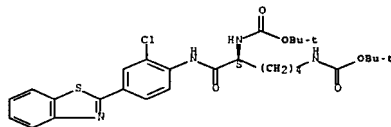
RN 328087-34-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



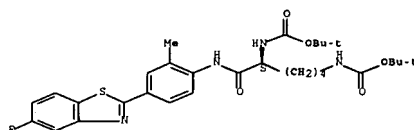
RN 398478-08-5 HCAPLUS  
 CN Carbamic acid, [(1S)-1-[[[4-(2-benzothiazolyl)-2-chlorophenyl]amino]carbonyl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



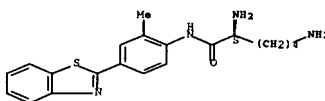
RN 398478-09-6 HCAPLUS  
 CN Carbamic acid, [(1S)-1-[[[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]amino]carbonyl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 398478-10-9 HCAPLUS  
 CN Carbamic acid, [(1S)-1-[[[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]amino]carbonyl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

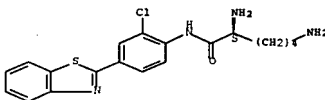
Absolute stereochemistry.



● 2 HCl

RN 328087-35-0 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-chlorophenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

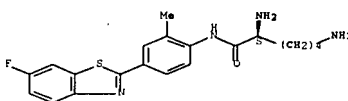
Absolute stereochemistry.



● 2 HCl

RN 328087-39-4 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

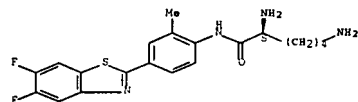
Absolute stereochemistry.



● 2 HCl

RN 328087-50-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(5,6-difluoro-2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

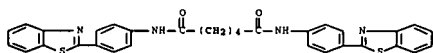
Absolute stereochemistry.



●2 HCl

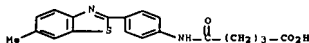
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2001:478094 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 135:298147  
 TITLE: Biological evaluation of hepatitis C virus helicase inhibitors  
 AUTHOR(S): Phoon, C. W.; Ng, P. Y.; Ting, A. E.; Yeo, S. L.; Sim, M. M.  
 CORPORATE SOURCE: Medicinal and Combinatorial Chemistry Laboratory, Institute of Molecular and Cell Biology, 117609, Singapore  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(13), 1647-1650  
 CODEN: BMCLSS; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:298147  
 AB A small chemical library has been synthesized and assayed for inhibition of HCV helicase activity. This study provides the structure-activity relationship of the reported inhibitors, with emphasis placed on the aminophenylbenzimidazole moiety and the linkers. Our data highlight the importance of preserving the aminophenylbenzimidazole core and the hydrophobic linkers for biol. activity. The development of a robust HCV helicase assay is also described.  
 IT 367279-22-9P 367279-25-2P 367279-27-4P  
 367279-30-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PRSP (Preparation); USRS (Uses)  
 [preparation and biol. evaluation of hepatitis C virus helicase inhibitors]  
 RN 367279-22-9 HCAPLUS  
 CN Hexanediamide, N,N'-bis[4-(2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)



RN 367279-25-2 HCAPLUS  
 CN Hexanediamide, N,N'-bis[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)

group. In all three of these groups the carboxylate or its Me ester is linked to the aryl group through various lengths of methylene carbons and amide or cinnamide groups. Optimal activity was observed when the carboxyl group was separated from the aryl group by a linking structure of five atoms in length. Both a double bond and an amide moiety are well tolerated in the linking structure.  
 IT 154355-46-1P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PRSP (Preparation) (potential aldose reductase inhibitors based on minimal pharmacophore requirements)  
 RN 154355-46-1 HCAPLUS  
 CN Pentanoic acid, 5-[4-(6-methyl-2-benzothiazolyl)phenyl]amino]-5-oxo- (9CI) (CA INDEX NAME)

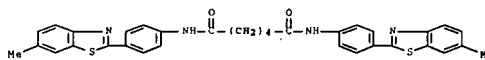


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

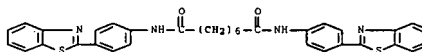
L9 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2001:152662 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 134:193429  
 TITLE: Preparation of substituted 2-phenylbenzothiazoles as antitumor agents  
 INVENTOR(S): Stevens, Malcolm Francis Graham; Poole, Tracey Dawn; Westwell, Andrew David; Hutchinson, Ian Paul; Chue, Mei-ze  
 PATENT ASSIGNEE(S): Cancer Research Campaign Technology Limited, UK  
 SOURCE: PCT Int. Appl., 58 pp.  
 CODEN: PIXX2D  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001014354	A1	20010301	WO 2000-GB3210	20000821
M: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TW, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SF, BJ, CP, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2382406	A1	20010301	CA 2000-2382406	20000821
EP 1204650	A1	20020515	EP 2000-954726	20000821
EP 1204650	B1	20060419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 200307462	T	20030225	JP 2001-518442	20000821
AU 783360	B2	20051020	AU 2000-67085	20000821
AT 323686	T	20060515	AT 2000-954726	20000821
PT 1204650	T	20060831	PT 2000-954726	20000821

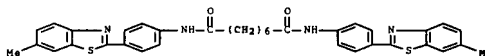
INDEX NAME)



RN 367279-27-4 HCAPLUS  
 CN Octanediamide, N,N'-bis[4-(2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)



RN 367279-30-9 HCAPLUS  
 CN Octanediamide, N,N'-bis[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)

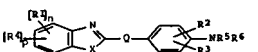


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2001:471832 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 135:226921  
 TITLE: Synthesis of potential aldose reductase inhibitors based on minimal pharmacophore requirements  
 AUTHOR(S): Schlitzer, Martin; Rodriguez, Labaniel; Kador, Peter F.  
 CORPORATE SOURCE: Institut für Pharmazeutische Chemie, Philipps-Universität Marburg, Marburg, D-35032, Germany  
 SOURCE: Journal of Pharmacy and Pharmacology (2001), 53(6), 831-839  
 CODEN: JPPHAB; ISSN: 0022-3573  
 PUBLISHER: Pharmaceutical Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:226921  
 AB A series of 17 compounds was synthesized based on the premise that the minimal pharmacophore for aldose reductase inhibition requires the presence of both an aryl group and a polar group connected by a linking structure. Three groups of compounds were synthesized, the first possessing a 4-(6-methyl-2-benzothiazolyl)aniline or 2-aminobenzothiazole group as the aryl group, the second possessing a 2-naphthyl as the aryl group and the third possessing either a 2-phenyl-4-thiazolyl or 5-(2-nitrophenyl)-2-furanyl as the aryl

ES 2263483	T3	20061216	ES 2000-954726	20000821
US 6858633	B1	20050222	US 2002-69018	20020729
PRIORITY APPLN. INFO.:			GB 1999-19673	A 19990820
			GB 1998-19673	A 19990820
			WO 2000-GB3210	W 20000821

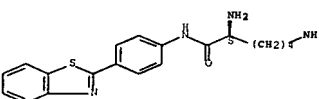
OTHER SOURCE(S): MARPAT 134:193429  
 GI



AB The title compds. [I; X = S, O; Q = a direct bond, CH2, CH=CH; R1 = halo, CF3, SnMe3; R2 = H, NO2, N3, etc.; R3 = H, halo, alkyl, etc.; R4 = alkyl, haloalkyl, OH, etc.; R5, R6 = H, amino acid residues, alkyl, etc.; p = 0-2; n = 0-3] which exhibit selective antiproliferative activity in respect of mammalian tumor cells, were prepared. E.g., a 4-step synthesis of I [X = S; Q = a direct bond; R1 = 4-F; R2 = 3-Me; R3-R6 = H] (starting with 3-methyl-4-nitrobenzoyl chloride and 2-fluoroaniline) which showed IC50 of <0.1 nM and of 0.13 nM in MCF-7 and MDA468 cell lines, resp., was given. At least in preferred compds. I the benzene ring of the benzothiazole nucleus has a halogen substituent, preferably fluorine, and the 2-Ph group has a 4'-amino substituent which may be conjugated with an amino acid to provide a water soluble amino acid amide prodrug or its salt.  
 IT 328087-33-8P 328087-34-9P 328087-35-0P  
 328087-38-3P 328087-39-4P 328087-50-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PRSP (Preparation); USRS (Uses)  
 [preparation of substituted 2-phenylbenzothiazoles as antitumor agents]

RN 328087-33-8 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)phenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

RN 328087-34-9 HCAPLUS  
 CN Hexanamide, 2,6-diamino-N-[4-(2-benzothiazolyl)-2-methylphenyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

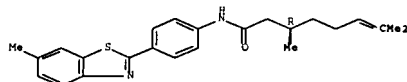
Absolute stereochemistry.



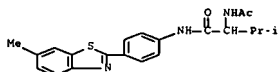


CN 4-Octenamide, 3,7-dimethyl-N-[4-(6-methyl-2-benzothiazolyl)phenyl]-, (3R)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 190436-44-3  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of (hetero)aromatic compds. for treating bone deficit conditions)  
RN 190436-44-3 HCAPLUS  
CN Butanamide, 2-(acetylamino)-3-methyl-N-[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1997:397336 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 127:17703  
TITLE: Preparation of (hetero)aromatic compounds for treating bone deficit conditions.  
INVENTOR(S): Petrie, Charles; Orme, Mark W.; Saundur, Nand; Robbins, Kirk G.; Harrie, Scott M.; Kontoyianni, Maria; Hurley, Laurence H.; Kerwin, Sean M.; Mundy, Gregory R.  
PATENT ASSIGNER(S): Zymogenetics, Inc., USA; Osteoscreen, Inc.; University of Texas At Austin  
SOURCE: PCT Int. Appl., 99 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

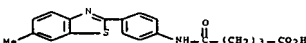
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9715308	A1	19970501	NO 1996-US17019	19961023
W: AL, AM, AU, BA, BB, BG, BR, CA, CN, CU, CZ, DE, FI, GE, HU, IL, IS, JP, KG, KP, KR, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, UZ, VN, AZ, BY, KZ, RU, TJ, TM, RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SF, BJ, CF, CG, CI, CM, GA, GN, ML,				

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 6  
PATENT INFORMATION:

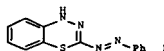
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9403811	A1	19940217	WO 1993-GB1628	19930802
W: CA, JP, US				
RM: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
GB 2270976	A	19940330	GB 1992-19743	19920918
GB 2260609	A	19930421	GB 1992-21578	19921014
GB 2260609	B	19960522		
GB 2261948	A	19930602	GB 1992-24897	19921127
GB 2261949	A	19930602	GB 1992-24898	19921127
EP 660935	A1	19950705	EP 1993-917968	19930802
EP 660935	B1	20000524		
R: DE, FR				
US 5723304	A	19980303	US 1995-381826	19950227
PRIORITY APPLN. INFO.:			GB 1992-16465	A 19920803
			GB 1992-19743	A 19920918
			GB 1992-20722	A 19921001
			GB 1992-21578	A 19921014
			GB 1992-24897	A 19921127
			GB 1992-24898	A 19921127
			GB 1991-22180	A 19911018
			GB 1991-25204	A 19911127
			GB 1991-25218	A 19911127
			NO 1993-GB1628	W 19930802

AB A method of detection, sensor, and test kit for immunoassays are described which involve radiometric detection of 2 detectable species which are detectable independently of one another and are influenced independently by the analyte. use an auxiliary ligand (e.g. an auxiliary antigen) and a binder (e.g. antibody) for the auxiliary ligand for radiometric detection of 2 detectable species. This improves the accuracy and precision of measurement of a signal by avoiding absolute measurements, e.g. where one of the detectable species is influenced by the presence of the analyte while the other is not, and the 2 detectable species can be detected independently. Thus, in an immunoassay for L-thyroxine, an antibody to thyroxine was conjugated with 5(6)-carboxyfluorescein N-hydroxysuccinimide ester. A 2nd antibody directed to 2-phenyl-4-quinolinecarboxylic acid was conjugated with thyroxine-N-amidoglutamic acid N-hydroxysuccinimide ester and with 7-amino-4-methylcoumarin-3-propionic acid N-hydroxysuccinimide ester. Polystyrene assay tubes coated with a 2-phenyl-4-quinolinecarboxylic acid-ovalbumin conjugate received standard solutions, or samples containing thyroxine and fluorescein-labeled primary antibody and then the 2nd antibody conjugate. After incubation and washing, the fluorescence bound to the tubes was measured at 510 nm (fluorescein) and 450 nm (7-amino-4-methylcoumarin). The fluorescence intensity for fluorescein increased with increasing thyroxine concentration, whereas that for the coumarin remained relatively constant. The ratios of the 2 fluorescence intensities was plotted as a function of thyroxine concentration for use as a calibration curve.

IT 154355-46-1  
RL: ANST (Analytical study)  
(as auxiliary ligand, in immunoassay with multiple label detection)  
RN 154355-46-1 HCAPLUS  
CN Pentanoic acid, 5-[(4-(6-methyl-2-benzothiazolyl)phenyl)amino]-5-oxo-  
(9CI) (CA INDEX NAME)

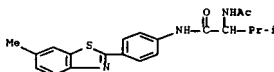


MR, NE, SN, TD, TO  
CA 2335481 A1 19970501 CA 1996-2235481 19961023  
AU 9674710 A 19970515 AU 1996-74710 19961023  
AU 706262 B2 19990610  
EP 866710 A1 19980930 EP 1996-936906 19961023  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IS, FI  
CN 1201393 A 19981209 CN 1996-197827 19961023  
HU 9802319 A2 19990201 HU 1998-2319 19961023  
BR 9611210 A 19991228 BR 1996-11210 19961023  
JP 2000513324 T 20001010 JP 1997-516761 19961023  
US 6008208 A 19991228 US 1997-878868 19970619  
NO 9801810 A 19980622 NO 1998-1810 19980422  
US 6413998 B1 20020702 US 1999-453828 19991202  
US 1995-5830P P 19951023  
US 1996-735875 B1 19961023  
WO 1996-US17019 W 19961023  
US 1997-878868 A3 19970619  
PRIORITY APPLN. INFO.:  
OTHER SOURCE(S): MARPAT 127:17703  
GI



AB A method for treating deficient bone growth and/or undesirable bone resorption comprises administration of compds. comprising 2 (substituted) aromatic systems spaced apart by a linker of 1.5-15 Å, is claimed. Thus, dithione was refluxed in EtOH/HOAc for 18 h to give 25% title compound (I). In a calvarial bone growth assay, I induced a 4-fold increase in width of new calvarial bone vs. controls.

IT 190436-44-3  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of (hetero)aromatic compds. for treating bone deficit conditions)  
RN 190436-44-3 HCAPLUS  
CN Butanamide, 2-(acetylamino)-3-methyl-N-[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)



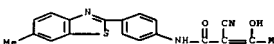
L9 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1994:239672 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 120:239672  
TITLE: Immunological detection using two detectable labels  
INVENTOR(S): Abukneesa, Ramadan Arbi  
PATENT ASSIGNER(S): GEC-Marconi Ltd., UK  
SOURCE: PCT Int. Appl., 61 pp.

L9 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1993:38708 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 118:38708  
TITLE: Novel immunosuppressive butenamides  
AUTHOR(S): Akton, Christopher A.; Billingham, Michael S. J.; Bishop, Paul M.; Gallagher, Peter T.; Hicks, Terence A.; Kitchen, E. Ann; Mullier, Graham W.; Owtan, W. Martin; Parry, Mark G.; et al.  
CORPORATE SOURCE: Lilly Res. Cent. Ltd., Windlesham/Surrey, GU20 6PH, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (17), 2203-13  
CODEN: JCPRB4; ISSN: 0300-922X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 118:38708  
GI

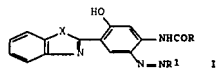
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 2-[4-(1,1-Dimethylethyl)phenyl]thiophene was carboxylated using butyllithium and carbon dioxide to give 5-[4-(1,1-dimethylethyl)phenyl]thiophene-2-carboxylic acid. Conversion of the acid using di-Ph phosphazide and triethylamine gave 5-[4-(1,1-dimethylethyl)phenyl]thiophene-2-carboxyl azide, which was rearranged in toluene at 110° with loss of nitrogen to give the isocyanate; this in turn was treated with sodium 1-cyanoprop-1-ene 2-oxide in THF to give 2-cyano-N-[5-[4-(1,1-dimethylethyl)phenyl]thiophen-2-yl]-3-hydroxybut-2-enamide (I). Analogous chemical has been utilized to synthesize both heteroarylphenylbutenamides, e.g., II and III and phenylbutenamides, e.g., IV (R = Cl, Bu, Me2CH, Me3C, EtMe2C, PrMe2C), which display immunosuppressive activity towards proliferating Con A-stimulated T-lymphocytes.

IT 145208-59-9  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and immunosuppressive activity of)  
RN 145208-59-9 HCAPLUS  
CN 2-Butenamide, 2-cyano-3-hydroxy-N-[4-(6-methyl-2-benzothiazolyl)phenyl]-  
(9CI) (CA INDEX NAME)



L9 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1985:186646 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 102:186646  
TITLE: Monoazo dyes for polyamide derived from 2-(4-alkylamido-2-hydroxyphenyl)benz-X-azoles  
AUTHOR(S): Barni, Rinaldo; Severino, Piero; Carpiagnano, Rosanna; Larovere, Raffaella; Girardo, Giacomo  
CORPORATE SOURCE: Ist. Chim. Org. Ind., Univ. Torino, Turin, 10125, Italy  
SOURCE: Dyes and Pigments (1985), 6(2), 83-97  
CODEN: DYPIDX; ISSN: 0143-7208



AB A series of 51 azo dyes (I: R = Me, Pr, n-C7H15, n-C11H23, n-C15H31; R1 = aryl; X = O, S, NH) derived from 2-(4-alkylamido-2-hydroxyphenyl)benz-X- azoles were prepared. The dyes were used as disperse dyes for polyamide fibers. Phys., chemical, spectroscopic and tech. properties of the dyes are discussed. A 'spectroscopic constant' is introduced to account for the color of dyes in solution and of dyed fabrics.

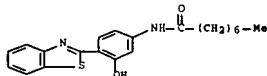
IT 88877-70-7 88877-71-8 88877-72-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling of, with diazotized anilines)

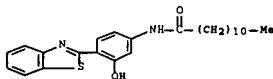
RN 88877-70-7 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]- (9CI) (CA INDEX NAME)



RN 88877-71-8 HCAPLUS

CN Dodecanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]- (9CI) (CA INDEX NAME)

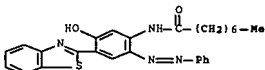


RN 88877-72-9 HCAPLUS

CN Hexadecanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]- (9CI) (CA INDEX NAME)

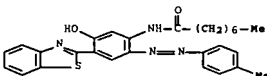
RN 95713-29-4 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-(phenylazo)phenyl]- (9CI) (CA INDEX NAME)



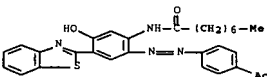
RN 95713-30-7 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(4-methylphenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



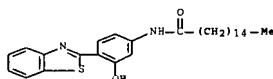
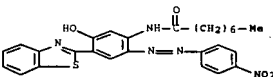
RN 95713-31-8 HCAPLUS

CN Octanamide, N-[2-[(4-acetylphenyl)azo]-4-(2-benzothiazolyl)-5-hydroxyphenyl]- (9CI) (CA INDEX NAME)



RN 95713-32-9 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(4-nitrophenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



IT 95713-03-4P 95713-04-5P 95713-05-6P

95713-29-4P 95713-30-7P 95713-31-8P

95713-32-9P 95713-33-0P 95713-34-1P

95713-35-2P 95713-36-3P 95713-37-4P

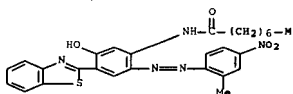
95713-38-5P 95713-39-6P 96743-27-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and dyeing properties on polyamide fibers)

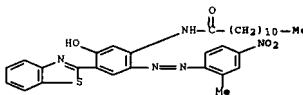
RN 95713-03-4 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(2-methyl-4-nitrophenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



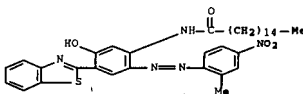
RN 95713-04-5 HCAPLUS

CN Dodecanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(2-methyl-4-nitrophenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



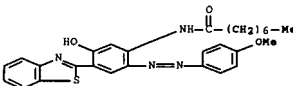
RN 95713-05-6 HCAPLUS

CN Hexadecanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(2-methyl-4-nitrophenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



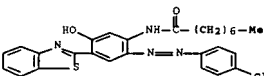
RN 95713-33-0 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(4-methoxyphenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



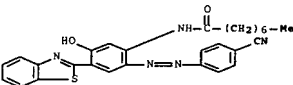
RN 95713-34-1 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-2-[(4-chlorophenyl)azo]-5-hydroxyphenyl]- (9CI) (CA INDEX NAME)



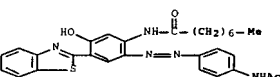
RN 95713-35-2 HCAPLUS

CN Octanamide, N-[4-(2-benzothiazolyl)-2-[(4-cyanophenyl)azo]-5-hydroxyphenyl]- (9CI) (CA INDEX NAME)



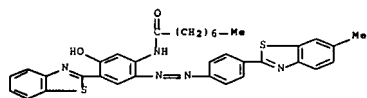
RN 95713-36-3 HCAPLUS

CN Octanamide, N-[2-[(4-(acetylamino)phenyl)azo]-4-(2-benzothiazolyl)-5-hydroxyphenyl]- (9CI) (CA INDEX NAME)

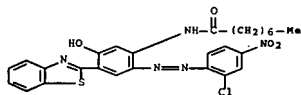


RN 95713-37-4 HCAPLUS

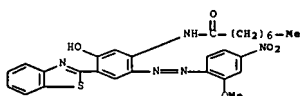
CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(4-(6-methyl-2-



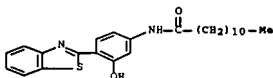
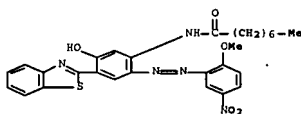
RN 95713-38-5 HCAPLUS  
CN Octanamide, N-[4-(2-benzothiazolyl)-2-[(2-chloro-4-nitrophenyl)azo]-5-hydroxyphenyl]- (9CI) (CA INDEX NAME)



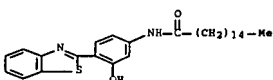
RN 95713-39-6 HCAPLUS  
CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(2-methoxy-4-nitrophenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



RN 96743-27-0 HCAPLUS  
CN Octanamide, N-[4-(2-benzothiazolyl)-5-hydroxy-2-[(2-methoxy-5-nitrophenyl)azo]phenyl]- (9CI) (CA INDEX NAME)



RN 88877-72-9 HCAPLUS  
CN Hexadecanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]- (9CI) (CA INDEX NAME)



L9 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1966:465965 HCAPLUS Full-text  
DOCUMENT NUMBER: 65:65965  
ORIGINAL REFERENCE NO.: 65:12316g-h,12317a-b  
TITLE: 4,4'-Dibenzamido-6,6'-alkylsulfonylstilbene-3,3'-disulfonic acids  
PATENT ASSIGNEE(S): J. R. Geigy A.-O.  
SOURCE: 11 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

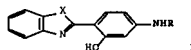
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1031750		19660602	GB 1964-51648	19641218
FR 1426394			CH	19631220

PRIORITY APPLN. INFO.:  
GI For diagram(s), see printed CA Issue.

AB Comps. of the general formula I are fluorescent brightening agents with improved chlorine fastness. Reduction of 4,2-CI(Me)C6H3SO2Cl with Na2SO3 gives 4,2-CI(Me)C6H3SO2H, methylated with Me2SO4 to give 4,2CI(Me)C6H3SO2Me (II), m. 70°. Nitration of II in H2SO4 gives 4,2,5-CI(Me)O2N)C6H2SO3Me, m. 137°, which, treated with Na2SO3, gives 5,2,4-MeO2N)C6H2SO3H, oxidized with aqueous NaOCl to [2,4,5-MeSO2(O2N)C6H2CH:12 (III) is reduced to [2,4,5-MeSO2(H2N)C6H2CH:12 (III). A suspension of 40 vols. III in 400 vols. anhydrous pyridine treated with a solution of 40 parts 4,2-MeO(C6H3COCl (IV) in 50 parts anhydrous PhMe, refluxed for 2 hrs. at 100-10°, treated with a solution of 40 parts IV in 50 parts PhMe, heated 2 hrs. at 100-10°, cooled, filtered, washed with C6H6, dried, stirred into 1200 parts 5% aqueous Na2CO3 at 70-80°, cooled, filtered, and washed with 2.5% aqueous NaCl gives I (X = OEt, Y = Me, Z = H). Similarly, other I are prepared (X, Y, and Z given): MeO, MeO, H; MeO, Me, Me; H, AcNH, H; H, EtO2CNH, H; HO, Me, H; HOCH2CH2O, Me, H; H, O2N, H; H, H2.

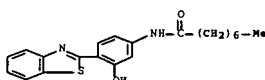
IT 10189-99-5p, 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, sodium salt (2CI)-90-5p, 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, sodium salt  
RL: PREP (Preparation)

L9 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1984:87237 HCAPLUS Full-text  
DOCUMENT NUMBER: 100:87237  
TITLE: 2-(4-Alkylamido-2-hydroxyphenyl)benz-X-azoles as intermediates for the synthesis of dyes  
AUTHOR(S): Barni, Ermanno; Savarino, Piero; Marzoni, Mario; Piva, Marco  
CORPORATE SOURCE: Ist. Chim. Org. Ind., Univ. Torino, Turin, Italy  
SOURCE: Journal of Heterocyclic Chemistry (1983), 20(6), 1517-21  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 100:87237  
GI



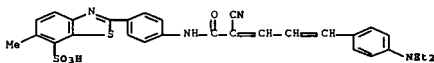
AB Nineteen substituted 2-phenylbenz-X-azoles (I; X = O, S, NH; R = H, C2-16 alkylcarbonyl) which are intermediates for the synthesis of dyes, were prepared from p-aminosalicylic acid [65-49-6]. The preferred route to the synthesis is discussed. The m.p.s. and the Rf values are correlated with the structure. An extensive discussion of the electronic absorption spectra, involving other comds. with the same general structure, is given.

IT 88877-70-7P 88877-71-8P 88877-72-9P  
RL: SPW (Synthetic preparation); PREP (Preparation)  
(preparation, electronic absorption spectrum and phys. properties of)  
RN 88877-70-7 HCAPLUS  
CN Octanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]- (9CI) (CA INDEX NAME)



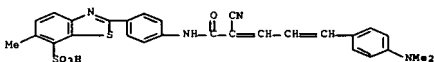
RN 88877-71-8 HCAPLUS  
CN Dodecanamide, N-[4-(2-benzothiazolyl)-3-hydroxyphenyl]- (9CI) (CA INDEX NAME)

(preparation of)  
RN 10189-99-5 HCAPLUS  
CN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido]phenyl]-6-methyl-, monosodium salt (8CI) (CA INDEX NAME)



● Na

RN 10210-90-9 HCAPLUS  
CN 7-Benzothiazolesulfonic acid, 2-[p-[2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido]phenyl]-7-methyl-, monosodium salt (8CI) (CA INDEX NAME)



● Na

L9 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1966:465964 HCAPLUS Full-text  
DOCUMENT NUMBER: 65:65964  
ORIGINAL REFERENCE NO.: 65:12316d-g  
TITLE: Substantive methine dyes  
INVENTOR(S): Cohen, Werner V.  
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.  
SOURCE: 5 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3257394		19660621	US 1962-218146	19620820
			US	19620820

PRIORITY APPLN. INFO.:  
GI For diagram(s), see printed CA Issue.

AB The title comds., aromatic sulfonic acids containing O groups as substituents, are greenish yellow dyes for paper which turn red on acidification. They are prepared by condensing 4-R(R')NC6H4CHO with cyanacetarilides. Thus, a mixture of [4,2-NCCCH2COHN(NaO3S)C6H3CH:12 5.5, 4-Me2NC6H4CHO 3.0, EtOH 16.0, and piperidine 0.15 part is heated at refluxing temperature for 3 hrs., cooled, filtered, washed with EtOH, and dried to give [4,2-Q(NaO3S)C6H3CH:12 (I, R = R' = Me, n = 0), bright green-yellow on paper pulp, green fluorescence under uv light, red on alum-treated paper, λH2Omax. 438 mμ, λMeOHmax. 418 mμ. Similarly, other I (n = 0) are prepared (R, R', λH2Omax. and λMeOHmax. and in mμ given): Et, CH2CH2OH, 448, 416; Et, CH2Ph, 440, 418. Similarly, x,1,3-Q(OH)C10H5SO3Na are

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prepared (x, R, R', n,  $\lambda$ 2Omax, and  $\lambda$ MOHmax, in  $\mu$  given): 6, Me, Me, 0, 436, 417; 6, Et, Et, 0, 443, 425; 6, Me, Et, 0, 439, 422; 6, Et, CH2CH2OH, 0, 436, 424; 6, Me, CH2CH2CN, 0, 418, 405; N, Et, CH2CH2CN, 0, 426, 412; 6, Et, CH2Ph, 0, 433, 412; 6, Me, CH2Ph, 0, 431, 410; 6, Et, CH2HCl, 0, 432, 410; 6, Me, Me, 1, 473, 460; 6, Et, Et, 1, 480, 470; 7, Me, Me, 0, 438, 424; 7, Et, Et, 0, 443, 422; 7, Et, CH2CH2OH, 0, 440, 423; 7, Me, Me, 1, 475, 462.

Similarly, 11 are prepared (R, R', n,  $\lambda$ 2O and  $\lambda$ 3OH, in m $\lambda$  given): Me, Me, 0, 447, 423; Et, Et, 0, 452, 430; Me, Et, 0, 450, 428; Et, CH2CH2OH, 0, 448, 427; Et, CH2Ph, 0, 438, 420; Me, Me, 1, 503, 466 (scarlet on paper); Et, Et, 1, 490, 487. Also prepared is 1,3,6-HO(NaO3S)C10H5NHCCO(CN):CHC6H3(NEt2)Me-4,2,  $\lambda$ 2Omax, 454 m $\lambda$ MeOHmax,  $\lambda$  436 m $\lambda$ . The dyes are soluble in HCONMe2, but only slightly soluble in H2O.

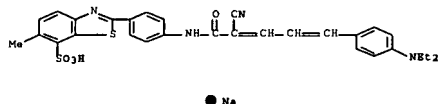
IT 10187-99-8P, 7-Benzothiazolesulfonic acid, 2-[p-(2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido)phenyl]-6-methyl-, sodium salt

10210-90-9P, 7-Benzothiazolesulfonic acid, 2-[p-(2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido)phenyl]-6-methyl-, sodium salt

RL: PREP (Preparation)

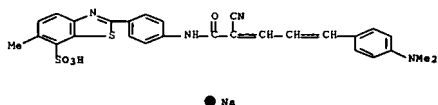
RN 10189-99-8 HCAPLUS

CN 7-Benzothiazolesulfonic acid, 2-[p-(2-cyano-5-[p-(diethylamino)phenyl]-2,4-pentadienamido)phenyl]-6-methyl-, monosodium salt (8CI) (CA INDEX NAME)



RN 10210-90-9 HCAPLUS

CN 7-Benzothiazolesulfonic acid, 2-[p-(2-cyano-5-[p-(dimethylamino)phenyl]-2,4-pentadienamido)phenyl]-7-methyl-, monosodium salt (8CI) (CA INDEX NAME)



=> file reg

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STRUCTURE FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2

DICTIONARY FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2

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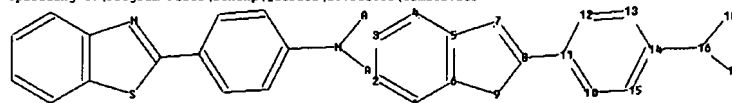
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> Uploading C:\Program Files\Stnexp\Queries\10.511852\clm16b.str



chain nodes : 16 18 19

ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds : 8-11 14-16 16-18 16-19

ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds : 5-7 7-8 14-16 16-18 16-19

exact bonds : 6-9 8-9 8-11

normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems : containing 1 : 10 :

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS 19:CLASS

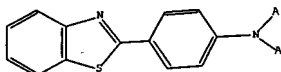
L10 STRUCTURE UPLOADED

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L10 HAS NO ANSWERS

L10 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 546 TO ITERATE

100.0% PROCESSED 546 ITERATIONS 23 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 9519 TO 12321

PROJECTED ANSWERS: 173 TO 747

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L13 432 L13 NOT L8

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L2 0 S 4992204/PA

L3 1 S US4992204/PN

FILE 'REGISTRY' ENTERED AT 14:28:06 ON 29 MAY 2007

FILE 'USPATFULL' ENTERED AT 14:28:12 ON 29 MAY 2007

TRA L3 1- RN : 74 TERMS

FILE 'REGISTRY' ENTERED AT 14:28:13 ON 29 MAY 2007

L4 74 SEA L4

L5 STRUCTURE UPLOADED

L6 4 S L6 SSS SAM

L7 127 S L6 SSS FULL

FILE 'HAPLUS' ENTERED AT 14:31:44 ON 29 MAY 2007

L9 24 S L8

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FILE 'REGISTRY' ENTERED AT 14:32:19 ON 29 MAY 2007

L10 STRUCTURE UPLOADED

L11 23 S L10 SSS SAM

L12 437 S L10 SSS FULL

L13 432 S L12 NOT L8

=> file hcaplus # l13

'S' IS AN AMBIGUOUS FILE OR CLUSTER NAME

SAFETY - Occupational Health and Safety Cluster

SBSESSION - Current files with L-numbers Cluster

STRUCTURE - Structure Searching Cluster

SUPPLIERS - Product Directories and Suppliers Cluster

SCISEARCH - ISI Science Citation Index from 1974 - present

SOLIDSTATE - Solid State and Superconductivity Abstracts from 1981

SOLIS - German literature in social sciences 1945-present

SPECINFO - Spectral Database Information System

STNGUIDE - Descriptive information about STN databases

STNMAIL - STN Electronic Mail Service

SYNTHLINE - Synthline Drug Synthesis Database 1984-present

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FULL ESTIMATED COST	176.15	500.16
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-18.72

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=> # l13

L14 568 L13

=> # l14 and py <2002

21897330 PY <2002

L15 388 L14 AND PY <2002

=> d ibib abs hitetr 1-10

L15 ANSWER 1 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:59558 HCAPLUS Full-text  
 DOCUMENT NUMBER: 140:127193  
 TITLE: Vaccines comprising aggregating protein epitopes and antibodies for treating a plaque-forming neurological or CNS disease  
 INVENTOR(S): Solomon, Beka; Frenkel, Dan  
 PATENT ASSIGNER(S): Ramot At Tel-Aviv University Ltd., Israel  
 SOURCE: U.S. Pat. Appl. Publ., 68 pp., Cont.-in-part of U.S. Ser. No. 162,889.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004013647	A1	20040122	US 2003-384788	20030311
US 6703015	B1	20040309	US 1999-473653	19991229
WO 2001018169	A2	20010315	WO 2000-11518	20000831

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6919075 B1 20050719 US 2001-830954 20000831  
 US 2002052311 A1 20020502 US 2001-808037 20010315  
 US 2003077252 A1 20030424 US 2002-162889 20020606  
 US 2004052766 A1 20040318 US 2003-618856 20030715  
 US 2005089510 A1 20050428 US 2004-749522 20040102  
 PRIORITY APPLN. INFO.: US 1999-152417P P 19990903  
 US 1999-473653 B2 19991229  
 US 2000-629971 B2 20000731  
 US 2001-830954 A2 20000831  
 WO 2000-11518 W 20000831  
 US 2001-808037 B2 20010315  
 US 2002-371735P P 20020412  
 US 2002-162889 A2 20020606

AB A method of immunizing against plaque forming diseases using display technol. is provided. The method utilize novel agents, or pharmaceutical compns. for vaccination against plaque forming diseases which rely upon presentation of an antigen or epitope on a display vehicle. The method further includes agents, or pharmaceutical compns. for vaccination against plaque forming diseases, which rely upon presentation of an antibody, or an active portion thereof, on a display vehicle. Whether antigens or antibodies are employed, disaggregation of plaques results from the immunization. The methods of the present invention also generally relates to treating and/or diagnosing neurol. diseases and disorders of the central nervous, regardless of whether the disease or disorder is plaque-forming or non-plaque forming.

IT 2390-54-7, Thioflavin  
 RL: ARU (Analytical role, unclassified); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)  
 (vaccines comprising aggregating protein epitopes and antibodies for diagnosis and treatment of plaque-forming neurol. or CNS disease)  
 RN 2390-54-7 HCAPLUS  
 CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
 (CA INDEX NAME)

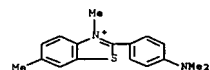
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:895600 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:34308  
 TITLE: Use of dimly fluorescing nucleic acid dyes in the identification of nucleated cells  
 INVENTOR(S): Hoffman, Robert A.; Frey, Thomas  
 PATENT ASSIGNER(S): Sention Dickinson and Company, USA  
 SOURCE: U.S., 7 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6329158	B1	20011211	US 1995-528828	19950915
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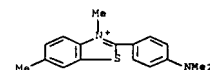
PRIORITY APPLN. INFO.:  
 AB This invention presents improved methodol. for identification of nucleated cells in flow cytometric anal. when immunofluorescent dyes are also used. Briefly, in the method nucleic acids are stained with a fluorescent dye which can then be used to identify the nucleated cells by measurement of fluorescence on a flow cytometer. The improvement presented by this invention is the use of a saturating (or near saturating) amount of a nucleic acid dye, or mixture of dyes, which gives low fluorescence at excitation conditions, so as not to greatly interfere with the signals of the immunofluorescent dyes.

IT 2390-54-7, Thioflavin T  
 RL: ARU (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (use of dimly fluorescing nucleic acid dyes in identification of nucleated cells)  
 RN 2390-54-7 HCAPLUS  
 CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
 (CA INDEX NAME)

• Cl<sup>-</sup>

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

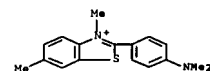
L15 ANSWER 4 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:843554 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:359238  
 TITLE: Photocatalytic paint containing pigment fading or discoloring by photocatalytic activity and method for coating using same  
 INVENTOR(S): Fujishima, Akira; Tada, Kaneyoshi  
 PATENT ASSIGNER(S): Kanagawa Academy of Science and Technology, Japan; Foundation for Scientific Technology Promotion  
 SOURCE: Jpn., Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent

• Cl<sup>-</sup>

L15 ANSWER 2 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:4680 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:158068  
 TITLE: Emission of thioflavin T and its off-on control in polymer membranes  
 AUTHOR(S): Raj, C. Retna; Ramaraj, R.  
 CORPORATE SOURCE: School of Chemistry, Madurai Kamaraj University, Madurai, 625021, India  
 SOURCE: Photochemistry and Photobiology (2001), 74(6), 752-759  
 CODEN: PHCBAP; ISSN: 0031-8655  
 PUBLISHER: American Society for Photobiology  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The absorption and emission spectral properties of thioflavin T (TFT+) in Nafion (NF) and cellulose matrices were studied. Formation of the emissive dimer is observed in both matrices. The monomer TFT+ emission is blueshifted in Nafion membrane (NF), whereas it is red shifted in cellulose membrane when compared with the emission in aqueous solution. The dimer emission of TFT+ in the Na+-NF membrane undergoes off-on switching with acids and alkalis. The TFT+ mol. undergoes protonation in the H+-NF and the protonated dye is fluorescent. The dimer emission of TFT+ is not observed in the dry H+-NF membrane because of the protonation of the TFT+ mol. The diffusion coefficient and the free energy of hydrophobic interaction for the TFT+ mol. in the NF membrane are calculated. The TFT+ mol. experiences hydrophobic and electrostatic interactions in the NF matrix, whereas it experiences a polar environment in the cellulose membrane. The 3-dimensional emission spectral studies support the formation of the emissive dimer in both NF and cellulose matrices.

IT 2390-54-7, Thioflavin T  
 RL: PRP (Properties)  
 (emission of thioflavin t and off-on control in polymer membranes)  
 RN 2390-54-7 HCAPLUS  
 CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
 (CA INDEX NAME)

• Cl<sup>-</sup>

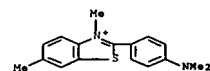
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS

LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001321676	A	20011120	JP 2000-144841	20000517
			JP 2000-144841	20000517

PRIORITY APPLN. INFO.:  
 AB The title paint contains a photocatalyst and a pigment which fade the color or discolors by the photocatalytic activity. The paint, which contains the pigment fading or discoloring by photocatalytic activity, provides the easy and precise detection of uneven coating thereof.

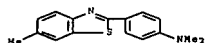
IT 2390-54-7, Thioflavin T  
 RL: TEM (Technical or engineered material use); USES (Uses)  
 (photocatalytic paint and method for coating using same)  
 RN 2390-54-7 HCAPLUS  
 CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
 (CA INDEX NAME)

• Cl<sup>-</sup>

L15 ANSWER 5 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:843336 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:115023  
 TITLE: Novel stilbenes as probes for amyloid plaques  
 AUTHOR(S): Kung, Hank F.; Lee, Chi-Man; Zhuang, Zhi-Ping; Kung, Mei-Ping; Hou, Catherine; Ploessel, Karl  
 CORPORATE SOURCE: Departments of Radiology and Pharmacology, University of Pennsylvania, Philadelphia, PA, 19104, USA  
 SOURCE: Journal of the American Chemical Society (2001), 123(50), 12740-12741  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Alzheimer's disease (AD) is a neurodegenerative disease of the brain characterized by dementia, cognitive impairment, and memory loss. Formation and accumulation of aggregates of  $\beta$ -amyloid (A $\beta$ ) peptides in the brain are critical factors in the development and progression of AD. The fibrillar aggregates of amyloid peptides, A $\beta$ 1-40 and A $\beta$ 1-42, are major metabolic peptides derived from amyloid precursor protein found in senile plaques and cerebrovascular amyloid deposits in AD patients. Our laboratory has reported two types of iodinated probes, styrylbenzenes (INSB) and thioflavins (benzothiazole, TZDM), for binding to A $\beta$  aggregates. In vitro binding studies of these ligands showed excellent binding affinities with Kd values of 0.13 and 0.06 nM for aggregates of A $\beta$ 1-40 and 0.73 and 0.14 nM for aggregates of A $\beta$ 1-42, resp. More importantly, under a competitive-binding assaying condition, two different and distinctive binding sites on A $\beta$ 1-40 and A $\beta$ 1-42 aggregates, which are mutually exclusive, were observed for styrylbenzenes (SB) and thioflavins (benzothiazole, TZ). Significantly, (125I)TZDM crossed intact blood-brain barrier and localized in the brain of normal mice after an i.v. injection. For in vivo imaging of A $\beta$  aggregates to succeed, it will be necessary to develop agents which show

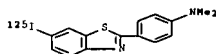
**10/511852** **93/217** **Robert Havlin**  
 good brain uptake in vivo. Brain penetration, a key factor for consideration, is usually related to the mol. size, neutrality, and lipophilicity. Further refinements of these probes are necessary to improve the brain uptake and washout from the normal brain regions and to achieve a high retention in the regions rich in A $\beta$  plaques.  
 IT 10205-62-6  
 RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)  
 (stilbenes as probes for amyloid plaques)  
 RN 10205-62-6 HCAPLUS  
 CN Benzenamine, N,N-dimethyl-4-(6-methyl-2-benzothiazolyl)- (CA INDEX NAME)



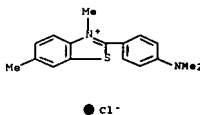
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:827673 HCAPLUS Full-text  
 DOCUMENT NUMBER: 137:59572  
 TITLE: IBOX (2-(4'-dimethylaminophenyl)-6-iodobenzoxazole): a ligand for imaging amyloid plaques in the brain  
 AUTHOR(S): Zhuang, Zhi-Ping; Kung, Mei-Ping; Hou, Catherine; Plesel, Karl; Skovronsky, Daniel; Gur, Tamar L.; Trojanowski, John Q.; Lee, Virginia M.-Y.; Kung, Hank P.  
 CORPORATE SOURCE: Department of Radiology, University of Pennsylvania, Philadelphia, PA, 19104, USA  
 SOURCE: Nuclear Medicine and Biology (2001), 28(8), 887-894  
 CODEN: NMBIO; ISSN: 0969-8051  
 PUBLISHER: Elsevier Science Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB It is well known that overprod. and accumulation of  $\beta$ -amyloid (A $\beta$ ) plaques in the brain is a key event in the pathogenesis of Alzheimer's disease (AD). Previously it was demonstrated that [125I]TZDM, 2-(4'-dimethylaminophenyl)-6-iodobenzothiazole, a thioflavin derivative, was an effective ligand with good in vitro and in vivo binding characteristics. To further improve the initial uptake and washout rate from the brain, important properties for in vivo imaging agents, a novel radioiodinated ligand, 2-(4'-dimethylaminophenyl)-6-iodobenzoxazole ([125I]IBOX), for detecting A $\beta$  plaques in the brain, was synthesized and evaluated. The new iodinated ligand, IBOX, is based on an isosteric replacement of a sulfur atom of TZDM by an oxygen, by which the mol. weight is reduced while the lipophilicity of the iodinated ligand is increased. Partition coeff. (P.C.) of these two ligands were 70 and 124 for TZDM and IBOX, resp. In vitro binding study indicated that the isosteric displacement yielded a new ligand with equal binding potency to A $\beta$ (1-40) aggregates (K<sub>i</sub> = 1.9 and 0.8 nM for TZDM and IBOX, resp.). Autoradiog. of postmortem brain sections of a confirmed AD patient by [125I]IBOX showed excellent labeling of plaques similar to that observed with [125I]TZDM. More importantly, in vivo biodistribution of [125I]IBOX in normal mice displayed superior peak brain uptake (2.08% at 30 min vs 1.57% at 60 min dose/brain for [125I]IBOX and [125I]TZDM, resp.). In addition, the washout from the brain was much faster for [125I]IBOX as compared to [125I]TZDM. Based on the data presented for [125I]IBOX, it is predicted that the brain trapping of this new radioiodinated ligand in the A $\beta$  containing regions will be more favorable than that of the parent compound, [125I]TZDM. Further evaluation of [125I]IBOX is warranted to confirm the A $\beta$  plaque labeling properties in vivo.  
 IT 346691-96-1  
 RL: DGN (Diagnostic use); PKT (Pharmacokinetics); BIOL (Biological study);

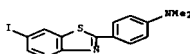
**10/511852** **94/217** **Robert Havlin**  
 USES (Uses)  
 (radioiodinated (dimethylaminophenyl)iodobenzoxazole for imaging amyloid plaques in brain: comparison with [125I]TZDM)  
 RN 346691-96-1 HCAPLUS  
 CN Benzenamine, 4-(6-iodo-2-benzothiazolyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



IT 2390-54-7, Thioflavin T 346691-94-9  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (radioiodinated (dimethylaminophenyl)iodobenzoxazole for imaging amyloid plaques in brain: effect of thioflavins on [125I]TZDM binding)  
 RN 2390-54-7 HCAPLUS  
 CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)



RN 346691-94-9 HCAPLUS  
 CN Benzenamine, 4-(6-iodo-2-benzothiazolyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:792340 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:331672  
 TITLE: Preparation of methionine derivatives as inhibitors of protein isoprenyl transferases  
 INVENTOR(S): Sebt, Said M.; Hamilton, Andrew D.; Augeri, David J.; Barr, Kenneth J.; Pakhoury, Stephen A.; Janowick, David A.; Kalvin, Douglas M.; O'Connor, Stephen J.; Rosenberg, Saul H.; Shen, Wang; Swenson, Rolf E.;

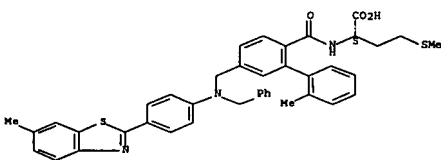
**10/511852** **95/217** **Robert Havlin**  
 Sorenson, Bryan K.; Sullivan, Gerard M.; Tasker, Andrew S.; Masioka, James T.; Nelson, Lissa T. J.; Henry, Kenneth J.; Wang, L.  
 PATENT ASSIGNEE(S): University of Pittsburgh, USA  
 SOURCE: U.S., 514 pp., Cont.-in-part of U.S. Ser. No. 852,858, abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 8  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6310095	B1	20011030	US 1998-73794	19980507 --
ZA 9906763	A	20000515	ZA 1999-6763	19991027 --
PRIORITY APPLN. INFO.:			US 1995-7247P	P 19951106
			US 1996-740909	B2 19961105
			US 1997-852858	B2 19970507
			US 1998-73794	A 19980507
			US 1998-197279	A 19981120

OTHER SOURCE(S): MARPAT 135:331672  
 AB Compd. R3-Z-L1-aryl [aryl is a benzene ring having certain substituents R1, R2, R4; L1 is LANR5L5 where L4 and L5 are absent or alkylene, R5 is H, alkanoyl, alkoxy, alkoxyalkyl, haloalkyl, etc.; Z is a covalent bond; R3 = cycloalkyl, alkoxy, alkyl, halogen, oxo, etc.] or their pharmaceutically acceptable salts, were prepared as inhibitors of protein isoprenyl transferases. Thus, N-[4-((R)-thiazolidin-4-ylcarbonyl)amino]-2-phenylbenzoyl]methionine Me ester hydrochloride, prepared via amidation reaction, showed 94% inhibition of farnesyl transferase at 1x10<sup>-6</sup> M.

IT 216233-18-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of methionine deriva. as inhibitors of protein isoprenyl transferases)  
 RN 216233-18-0 HCAPLUS  
 CN L-Methionine, N-[[2'-methyl-5-[[[4-(6-methyl-2-benzothiazolyl)phenyl](phenylmethyl)amino]methyl][1,1'-biphenyl]-2-yl]carbonyl]-, monolithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

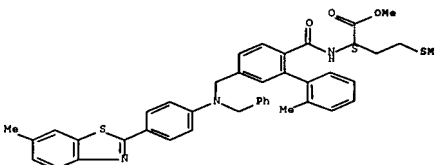


● Li

IT 216233-23-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

**10/511852** **96/217** **Robert Havlin**  
 (preparation of methionine deriva. as inhibitors of protein isoprenyl transferases)  
 RN 216233-23-1 HCAPLUS  
 CN L-Methionine, N-[[2'-methyl-5-[[[4-(6-methyl-2-benzothiazolyl)phenyl](phenylmethyl)amino]methyl][1,1'-biphenyl]-2-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



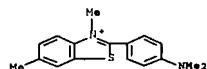
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:784637 HCAPLUS Full-text  
 DOCUMENT NUMBER: 137:30072  
 TITLE: Amyloid fibril formation in microwell plates for screening of inhibitors  
 AUTHOR(S): Lin, Yuh-Mei; Raffin, Rosemarie; Zhou, Yasheen; Cassidy, Constance S.; Flavin, Michael T.; Stevens, Fred J.  
 CORPORATE SOURCE: MediChem Life Sciences, Inc., Woodridge, IL, 60517, USA  
 SOURCE: Amyloid (2001), 8(3), 182-193  
 CODEN: AIJIRT; ISSN: 1350-6129  
 PUBLISHER: Parthenon Publishing Group  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Fibril formation is the basis of amyloid production in a number of disease states, such as Alzheimer's disease, diabetes and immunocytic dyscrasias. Compd. that inhibit fibril formation could be directly relevant to the treatment of amyloid diseases, and may also provide a foundation for the development of interventions in other mol. condensation diseases ranging from sickle cell anemia to atherosclerosis. We developed an economical and convenient high-throughput method for screening compds. against fibril formation in microwell plates. Chalcones, flavonoids and biflavonoids were screened against fibril formation by a recombinant antibody variable domain (VL). Chalcones 6 and 14 were found to demonstrate inhibition at 0.1  $\mu$ M in 79  $\mu$ M of protein solution in both test tube and microwell plate assays. The concentration of protein in the microwell plate assay could be as low as 5  $\mu$ M using ThT as a monitoring agent. Mol. modeling studies indicated that both compds. could be individually docked into a binding site at the monomer-monomer interface of the VL protein dimer. These studies suggested that these compds. could potentially stabilize the VL dimer and therefore reduce its tendency to form fibrils. These findings may provide the basis for a new therapeutic approach to prevent or treat amyloid diseases.

IT 2390-54-7, Thioflavin T  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (amyloid fibril formation in microwell plates for screening of inhibitors)

RN 2390-54-7 HCAPLUS  
CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
(CA INDEX NAME)

● Cl<sup>-</sup>

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 388 HCAPLUS COPYRIGHT 2007 ACS ON STM  
ACCESSION NUMBER: 2001:763055 HCAPLUS Full-text  
DOCUMENT NUMBER: 135:1313600  
TITLE: Methods of investigating, diagnosing, and treating amyloidosis  
INVENTOR(S): Solomon, Alan; Wall, Jonathan; Hrnec, Rudi; Schell, Maria  
PATENT ASSIGNEE(S): University of Tennessee Research Corporation, USA  
SOURCE: PCT Int. Appl., 57 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077167	A2	20011018	WO 2001-US11043	20010405
WO 2001077167	A3	20030828		

M: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DS, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

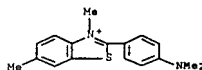
RM: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TO

CA 2404237	A1	20011018	CA 2001-2404237	20010405
US 2002019335	A1	20020214	US 2001-825872	20010405
EP 1353944	A2	20031022	EP 2001-926636	20010405

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR

PRIORITY APPLN. INFO.: US 2000-194684P P 20000405  
WO 2001-US11043 W 20010405  
AB The present invention provides a therapeutic method for removing amyloid fibrils from a patient. The present invention also provides a transgenic animal that develops systemic AA amyloidosis within three weeks for use as a tool to investigate AA amyloidosis and to evaluate agents that may be potentially useful in preventing and treating amyloid-related disorders. Further, the present invention provides diagnostic assays for monitoring Ig light chain fibrillogenesis in real-time and for identification of the chemical nature of

the protein in amyloid deposits which enables the determination of the type of amyloidosis for therapeutic and prognostic purposes.  
IT 2390-54-7, Thioflavin T  
RL: ARG (Analytical reagent use); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
(method of investigating and diagnosing and treating amyloidosis)  
RN 2390-54-7 HCAPLUS  
CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
(CA INDEX NAME)

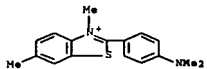
● Cl<sup>-</sup>

L15 ANSWER 10 OF 388 HCAPLUS COPYRIGHT 2007 ACS ON STM  
ACCESSION NUMBER: 2001:612449 HCAPLUS Full-text  
DOCUMENT NUMBER: 135:328800  
TITLE: Uncharged thioflavin-T derivatives bind to amyloid-beta protein with high affinity and readily enter the brain  
AUTHOR(S): Klunk, William S.; Wang, Yanming; Huang, Guo-Feng; Debnath, Manik L.; Holt, Daniel P.; Mathis, Chester A.  
CORPORATE SOURCE: Laboratory of Molecular Neuropharmacology, Department of Psychiatry, University of Pittsburgh School of Medicine, Pittsburgh, PA, 15213, USA  
SOURCE: Life Sciences (2001), 69(13), 1471-1484  
CODEN: LIFBAA; ISSN: 0024-3205  
PUBLISHER: Elsevier Science Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

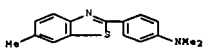
AB In vivo assessment of the beta-sheet proteins deposited in amyloid plaques (Aβ peptide) or neurofibrillary tangles (tau protein) presents a target for the development of biol. markers for Alzheimer's disease (AD). In an effort to develop in vivo beta-sheet imaging probes, derivs. of thioflavin-T (ThT) were synthesized and evaluated. These compds. lack the pos. charged quaternary heterocyclic nitrogen of ThT and are therefore uncharged at physiol. pH. They are 600-fold more lipophilic than ThT. These ThT derivs. bind to Aβ(1-40) fibrils with higher affinity (K<sub>i</sub> = 20.2 nM) than ThT (K<sub>i</sub> = 890 nM). The uncharged ThT derivs. stained both plaques and neurofibrillary tangles in post-mortem AD brain, showing some preference for plaque staining. A carbon-11 labeled compound, [N-methyl-11C]6-Me-BTA-1, was prepared, and its brain entry and clearance were studied in Swiss-Webster mice. This compound entered the brain at levels comparable to commonly used neuroreceptor imaging agents (0.223% ID/kg or 7.61% ID/g at 2 min post-injection) and showed good clearance of free and non-specifically bound radioactivity in normal rodent brain tissue (brain clearance t<sub>1/2</sub> = 20 min). The combination of relatively high affinity for amyloid, specificity for staining plaques and neurofibrillary tangles in post-mortem AD brain, and good brain entry and clearance makes [N-methyl-11C]6-Me-BTA-1 a promising candidate as an in vivo positron emission tomog. (PET) beta-sheet imaging agent.

IT 2390-54-7, Thioflavin-T  
RL: PRP (Properties)  
(uncharged thioflavin-T derivs. bind to amyloid-beta protein and enter brain)  
RN 2390-54-7 HCAPLUS  
CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)

(CA INDEX NAME)

● Cl<sup>-</sup>

IT 10205-62-6P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(uncharged thioflavin-T derivs. bind to amyloid-beta protein and enter brain)  
RN 10205-62-6 HCAPLUS  
CN Benzenamine, N,N-dimethyl-4-(6-methyl-2-benzothiazolyl)- (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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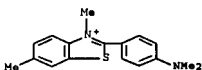
L15 ANSWER 11 OF 388 HCAPLUS COPYRIGHT 2007 ACS ON STM  
ACCESSION NUMBER: 2001:552957 HCAPLUS Full-text  
DOCUMENT NUMBER: 135:131425  
TITLE: Test strip for detecting elevated amounts of chloride in swimming pools and thermal stations  
INVENTOR(S): Rupasingh Lakshman, Fernando S.; Kreiser, Liese  
PATENT ASSIGNEE(S): Environmental Test Systems, Inc., USA  
SOURCE: Fr. Demande, 17 pp.  
CODEN: FRXXBL  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2800166	A1	20010427	FR 2000-13374	20001019
CA 2321954	A1	20010420	CA 2000-2321954	20001019
ES 2172432	A1	20020916	ES 2000-2506	20001019
ES 2172432	B1	20031216		

PRIORITY APPLN. INFO.: US 1999-420995 A 19991020  
AB A non-instrumental rapid visual method for detection of chloride ions over a large concentration interval, especially in swimming pool water, is based on a rapid reaction with a colorimetric indicator at pH 0.2-2.5 with the water in the presence of a reagent containing: (1) a silver complex of 2,4,6-tris(2-pyridyl)-1,3,5-triazine, (2) a stable source of chloride-free ferrous ion, (3) a citric acid buffer, and (4) a yellow color

indicator based on thioflavine-T. The intensity of the color is then compared with that of reference solns. containing a known concentration (at the ppm level) of chloride.

IT 2390-54-7, Thioflavine-T  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(indicator: test strip for detecting elevated amts. of chloride in swimming pools and thermal stations)  
RN 2390-54-7 HCAPLUS  
CN Benzoethiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
(CA INDEX NAME)

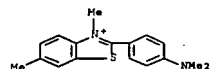
● Cl<sup>-</sup>

L15 ANSWER 12 OF 388 HCAPLUS COPYRIGHT 2007 ACS ON STM  
ACCESSION NUMBER: 2001:501015 HCAPLUS Full-text  
DOCUMENT NUMBER: 135:207387  
TITLE: Thioflavin T is a fluorescent probe of the acetylcholinesterase peripheral site that reveals conformational interactions between the peripheral and acylation sites  
AUTHOR(S): De Ferrari, Giancarlo V.; Mallender, William D.; Inestrosa, Nibaldo C.; Rosenberry, Terrone L.  
CORPORATE SOURCE: Centro de Regulacion Celular y Patologica, Departamento de Biologia Celular y Molecular, Facultad de Ciencias Biologicas, Pontificia Universidad Catolica de Chile, Santiago, 114-D, Chile  
SOURCE: Journal of Biological Chemistry (2001), 276(26), 23282-23287  
CODEN: JBCHA3; ISSN: 0021-9258  
PUBLISHER: American Society for Biochemistry and Molecular Biology  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Three-dimensional structures of acetylcholinesterase (AChE) reveal a narrow and deep active site gorge with two sites of ligand binding, an acylation site at the base of the gorge, and a peripheral site near the gorge entrance. Recent studies have shown that the peripheral site contributes to catalytic efficiency by transiently binding substrates on their way to the acylation site, but the question of whether the peripheral site makes other contributions to the catalytic process remains open. A possible role for ligand binding to the peripheral site that has long been considered is the initiation of a conformational change that is transmitted allosterically to the acylation site to alter catalysis. However, evidence for conformational interactions between these sites has been difficult to obtain. Here we report that thioflavin T, a fluorophore widely used to detect amyloid structure in proteins, binds selectively to the AChE peripheral site with an equilibrium dissociation constant of 1.0 μM. The fluorescence of the bound thioflavin T is increased more than 1000-fold over that of unbound thioflavin T, the greatest enhancement of fluorescence for the binding of a fluorophore to AChE yet observed. Furthermore, when the acylation site ligands edrophonium or m-(N,N,N-trimethylammonio)trifluoroacetophenone form ternary complexes with AChE and thioflavin T, the fluorescence is quenched by factors of 2.7-4.2. The observation of this partial quenching of thioflavin T fluorescence is a major advance in the study of AChE for two reasons. First, it allows thioflavin T to be used as a reporter for ligand reactions at



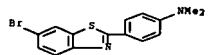
the acylation site. Second, it indicates that ligand binding to the acylation site initiates a change in the local ACHS conformation at the peripheral site that quenches the fluorescence of bound thioflavin T. The data provide strong evidence in support of a conformational interaction between the two ACHS sites.

IT 2390-54-7, Thioflavin T  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
 (thioflavin T is a fluorescent probe of acetylcholinesterase peripheral site that reveals conformational interactions between peripheral and acylation sites)  
 RN 2390-54-7 HCAPLUS  
 CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)

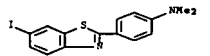


REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

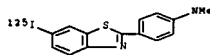
L15 ANSWER 13 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:383781 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:86478  
 TITLE: Study of  $\gamma$ -irradiated benzothiazole-doped polyvinyl chloride by positron annihilation  
 AUTHOR(S): Misheva, M.; Djourellov, N.; Sertova, N.; Petkov, I.; Deligeorgiev, T.  
 CORPORATE SOURCE: Faculty of Physics, Sofia University, Sofia, BG-1126, Bulg.  
 SOURCE: Materials Science Forum (2001), 363-365 (Positron Annihilation), 319-321  
 CODEN: MSFOEP; ISSN: 0255-5476  
 PUBLISHER: Trans Tech Publications Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Poly(vinyl chloride) (PVC) films containing 0-4 weight% of 2-(p-dimethylaminophenyl)benzothiazole (BT) are studied by positron lifetime and Doppler broadening of annihilation line measurements. The effects of gamma-irradiation dose and of BT contents on positron annihilation parameters are studied. The positron lifetimes and intensities depend on irradiation dose only for BT-doped films. The ortho-positronium intensities for pure and doped PVC decrease with dose increasing in a similar way. The influence of doping is significant only at first doping with 0.125 wt% BT and is weak afterwards. Some of the observed changes of the parameters are explained by the protonation of BT and its conversion into [BT $\cdot$ Cl $^-$ ] complexes by the interaction with hydrogen chloride - a product of PVC photodegradn.  
 IT 10205-56-8, 2-(p-Dimethylaminophenyl)benzothiazole  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (gamma-irradiated (dimethylaminophenyl)benzothiazole-doped PVC studied by positron annihilation)  
 RN 10205-56-8 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-dimethyl- (CA INDEX NAME)



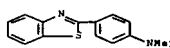
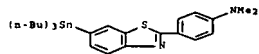
IT 346691-94-9P  
 RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)  
 (preparation of radioiodinated styrylbenzenes and thioflavins for amyloid aggregate imaging)  
 RN 346691-94-9 HCAPLUS  
 CN Benzenamine, 4-(6-iodo-2-benzothiazolyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



IT 346691-96-1P  
 RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
 (preparation of radioiodinated styrylbenzenes and thioflavins for amyloid aggregate imaging)  
 RN 346691-96-1 HCAPLUS  
 CN Benzenamine, 4-[6-(iodo-125I)-2-benzothiazolyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



IT 346691-92-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of radioiodinated styrylbenzenes and thioflavins for amyloid aggregate imaging)  
 RN 346691-92-7 HCAPLUS  
 CN Benzenamine, N,N-dimethyl-4-[6-(tributylstannyl)-2-benzothiazolyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:315921 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:73471  
 TITLE: Radioiodinated Styrylbenzenes and Thioflavins as Probes for Amyloid Aggregates  
 AUTHOR(S): Zhuang, Z.-P.; Kung, M.-P.; Hou, C.; Skovronsky, D. M.; Gur, T. L.; Ploessl, K.; Trojanowski, J. Q.; Lee, V. M.-Y.; Kung, H. F.  
 CORPORATE SOURCE: Departments of Radiology Pathology and Laboratory Medicine and Pharmacology, University of Pennsylvania, Philadelphia, PA, 19104, USA  
 SOURCE: Journal of Medicinal Chemistry (2001), 44(12), 1905-1914  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB We report for the first time that small mol.-based radioiodinated ligands, showing selective binding to A $\beta$  aggregates, cross the intact blood-brain barrier by simple diffusion. Four novel ligands showing preferential labeling of amyloid aggregates of A $\beta$ (1-40) and A $\beta$ (1-42) peptides, commonly associated with plaques in the brain of people with Alzheimer's disease (AD), were developed. Two 125I-labeled styrylbenzenes, (E,S)-1-iodo-2,5-bis(3-hydroxycarbonyl-4-hydroxy)styrylbenzene, I (ISS), and (E,S)-1-iodo-2,5-bis(3-hydroxycarbonyl-4-methoxy)styrylbenzene, II (IMSB), and two 125I-labeled thioflavins, 2-[4-(dimethylamino)phenyl]-6-iodobenzothiazole, III (TZDM), and 2-[4-(4'-methylypiperazin-1-yl)phenyl]-6-iodobenzothiazole, IV (TZPI), were prepared at a high specific activity (200 Ci/mmol). In vitro binding studies of these ligands showed excellent binding affinities with Kd values of 0.08, 0.13, 0.06, and 0.13 nM for aggregates of A $\beta$ (1-40) and 0.15, 0.73, 0.14, and 0.15 nM for aggregates of A $\beta$ (1-42), resp. Interestingly, under a competitive-binding assaying condition, different binding sites on A $\beta$ (1-40) and A $\beta$ (1-42) aggregates, which are mutually exclusive, were observed for styrylbenzenes and thioflavins. Autoradiog. studies of postmortem brain sections of a patient with Down's syndrome known to contain primarily A $\beta$ (1-42) aggregates in the brain showed that both [125I]-III and [125I]-IV labeled these brain sections, but [125I]-II, selective for A $\beta$ (1-40) aggregates, exhibited very low labeling of the comparable brain section. Biodistribution studies in normal mice after an iv injection showed that [125I]-III and [125I]-IV exhibited excellent brain uptake and retention, the levels of which were much higher than those of [125I]-I and [125I]-II. These findings strongly suggest that the new radioiodinated ligands may be useful as biomarkers for studying A $\beta$ (1-40) as well as A $\beta$ (1-42) aggregates of amyloidogenesis in AD patients.

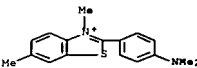
IT 346691-88-1P  
 RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation of radioiodinated styrylbenzenes and thioflavins for amyloid aggregate imaging)  
 RN 346691-88-1 HCAPLUS  
 CN Benzenamine, 4-(6-bromo-2-benzothiazolyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 15 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:315233 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:16316  
 TITLE: The relationship between A $\beta$ -associated free radical generation and A $\beta$  fibril formation revealed by negative stain electron microscopy and thioflavine-T fluorometric assay  
 AUTHOR(S): Monji, A.; Utsuni, H.; Yoshida, I.; Hashikawa, S.; Tashiro, K.-i.; Tashiro, N.  
 CORPORATE SOURCE: Graduate School of Medical Sciences, Department of Neuropsychiatry, Kyushu University, Fukuoka, 812-8582, Japan  
 SOURCE: Neuroscience Letters (2001), 304(1-2), 65-68  
 CODEN: NELEDS; ISSN: 0304-3940  
 PUBLISHER: Elsevier Science Ireland Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB In the present study, we investigated whether or not the A $\beta$  peptide itself spontaneously generates free radicals using ESR (ESR) spectroscopy while also observing the A $\beta$  fibril formation by neg. stain electron microscopy. The present results demonstrated a four-line spectrum in the presence of A $\beta$ (1-40) with N-tert-butyl- $\alpha$ -phenylnitron (PBN) but not in the presence of PBN alone in phosphate-buffered saline. Neg. stain electron microscopy has shown that A $\beta$  peptides after 96 h of incubation showed more amyloid-like fibrils than those after 72 h of incubation while the four-line spectrum obtained by ESR spectroscopy attained a maximum intensity after 72 h of incubation and thereafter its intensity immediately decreased during the 4-day incubation period. These results were also supported by a thioflavine-T (Th-T) fluorometric assay. In conclusion, the present results suggest that A $\beta$ -associated free radical generation is correlated with A $\beta$  fibril formation while its generation is only observed transiently during the process of A $\beta$  fibril formation.

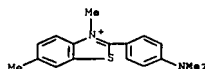
IT 2390-54-7, Thioflavine-T  
 RL: ANT (Analyte); ANST (Analytical study)  
 (A $\beta$ -associated free radical generation and A $\beta$  fibril formation relationship revealed by neg. stain electron microscopy and thioflavine-T fluorometric assay)  
 RN 2390-54-7 HCAPLUS  
 CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 16 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:313329 HCAPLUS Full-text

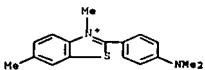
10/511852 105/217 Robert Havlin  
DOCUMENT NUMBER: 135/42183  
TITLE: Sepiolite-based materials for the photo- and thermal-stabilization of pesticides  
AUTHOR(S): Casal, B.; Merino, J.; Serratos, J.-M.; Ruiz-Hitzky, S.  
CORPORATE SOURCE: Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, Madrid, E-28049, Spain  
SOURCE: Applied Clay Science (2001), 18(5-6), 245-254  
CODEN: ACLSER; ISSN: 0169-1317  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The work is on the use of sepiolite for the stabilization of certain photo- or thermolabile herbicides by their adsorption on modified sepiolite that act as organo-inorg. supports. Formulations based on sepiolite containing a cationic dye (thioflavine-T) are very effective in the stabilization of a photolabile herbicide (trifluralin). A modification of the hydrophilic character of the sepiolite surface by adsorption of cationic surfactants enhances the adsorption on the mineral substrate of non-polar pesticides, such as the herbicides alachlor or metolachlor, thus contributing to the decrease of their losses by volatilization.  
IT 2390-54-7D, Thioflavine-T, sepiolite modifier  
RL: MCA (Modifier or additive use); PRP (Properties); USES (Uses)  
(modified sepiolite for the photo- and thermal stabilization of herbicides)  
RN 2390-54-7 HCAPLUS  
CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 17 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2001:282855 HCAPLUS Full-text  
DOCUMENT NUMBER: 134/361599  
TITLE: Effect of Environmental Factors on the Kinetics of Insulin Fibril Formation: Elucidation of the Molecular Mechanism  
AUTHOR(S): Nielsen, Liza; Khurana, Ritu; Coats, Alisa; Frokjaer, Sven; Brange, Jens; Vyas, Sandip; Uversky, Vladimir N.; Fink, Anthony L.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA, 95064, USA  
SOURCE: Biochemistry (2001), 40(20), 6036-6046  
CODEN: BICHAM; ISSN: 0006-2960  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB In the search for the mol. mechanism of insulin fibrillation, the kinetics of insulin fibril formation were studied under different conditions using the fluorescent dye

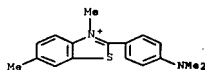
10/511852 107/217 Robert Havlin  
CR, CU, CZ, DE, DK, DM, DZ, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MY, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KS, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, ML, PT, SE, SF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
CA 2385123 A1 20010419 CA 2000-2385123 20001016 <--  
EP 1222203 A1 20020717 EP 2000-968122 20001016  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IS, SI, LT, LV, FI, RO, MK, CY, AL  
JP 2003512029 T 20030402 JP 2001-530370 20001016  
PRIORITY APPLN. INFO.: GB 1999-24484 A 19991015  
WO 2000-GB3974 W 20001016  
AB The present invention provides a method of designing a modified polypeptide having an altered tendency to aggregate compared to the unmodified polypeptide. The method comprises: analyzing the amino acid sequence of a predetd. polypeptide to determine the propensity of the polypeptide to form local structure; comparing the propensity to form local structure of a modified polypeptide to the propensity to form local structure of an unmodified polypeptide; and determining thereby whether the modified polypeptide has an altered tendency to aggregate in the denatured state relative to the unmodified polypeptide. A selected modified polypeptide having the altered tendency to aggregate is then produced. The invention also provides a method of producing a modified polypeptide having an altered tendency to aggregate compared to the unmodified polypeptide, which method comprises: (i) introducing at least one amino acid modification into a predetd. polypeptide sequence such that said modified polypeptide has an altered propensity to form local structure in the denatured state relative to the unmodified polypeptide, and optionally (ii) recovering the modified polypeptide, and/or optionally (iii) allowing the modified polypeptides to form an aggregate. Use of the method of altering protein aggregation in a method of treatment or diagnosis of an amyloid or aggregate associated disease is disclosed.  
IT 2390-54-7, Thioflavine T  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(aggregation kinetics measuring using; method of altering protein aggregation and therapeutic uses)  
RN 2390-54-7 HCAPLUS  
CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 19 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2001:275684 HCAPLUS Full-text  
DOCUMENT NUMBER: 135/72313  
TITLE: Promotion of formation of amyloid fibrils by aluminium adenosine triphosphate (AlATP)  
AUTHOR(S): Skley, C.; Korchazhkina, O. V.  
CORPORATE SOURCE: Birchall Centre for Inorganic Chemistry and Materials

10/511852 106/217 Robert Havlin  
thioflavin T (THT). The effect of insulin concentration, agitation, pH, ionic strength, anions, seeding, and addition of 1-anilinonaphthalene-8-sulfonic acid (ANS), urea, TMAO, sucrose, and THT on the kinetics of fibrillation was investigated. The kinetics of the fibrillation process could be described by the lag time for formation of stable nuclei (nucleation) and the apparent rate constant for the growth of fibrils (elongation). The addition of seeds eliminated the lag phase. An increase in insulin concentration resulted in shorter lag times and faster growth of fibrils. Shorter lag times and faster growth of fibrils were seen at acidic pH vs. neutral pH, whereas an increase in ionic strength resulted in shorter lag times and slower growth of fibrils. There was no clear correlation between the rate of fibril elongation and ionic strength. Agitation during fibril formation attenuated the effects of insulin concentration and ionic strength on both lag times and fibril growth. The addition of ANS increased the lag time and decreased the apparent growth rate for insulin fibril formation. The ANS-induced inhibition appears to reflect the formation of amorphous aggregates. The denaturant, urea, decreased the lag time, whereas the stabilizers, trimethylamine N-oxide dihydrate (TMAO) and sucrose, increased the lag times. The results indicated that both nucleation and fibril growth were controlled by hydrophobic and electrostatic interactions. A kinetic model, involving the association of monomeric partially folded intermediates, whose concentration is stimulated by the air-water interface, leading to formation of the critical nucleus and thence fibrils, is proposed.  
IT 2390-54-7, Thioflavin T  
RL: NUU (Other use, unclassified); USES (Uses)  
(environmental factors effect on kinetics of insulin fibril formation and mol. mechanism therein)  
RN 2390-54-7 HCAPLUS  
CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)

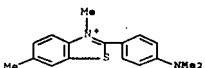


REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 18 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2001:283993 HCAPLUS Full-text  
DOCUMENT NUMBER: 134/307615  
TITLE: Method of altering protein aggregation and therapeutic uses  
INVENTOR(S): Villegas, Virtudes; Zurdo, Jesus; Aviles, Francesc; Dobson, Christopher Martin; Serrano, Luis  
PATENT ASSIGNER(S): Ise Innovation Limited, UK  
SOURCE: PCT Int. Appl., 87 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001027152	A1	20010419	WO 2000-GB3974	20001016 <--
W: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

10/511852 108/217 Robert Havlin  
SOURCE: Science, School of Chemistry and Physics, Keele University, Staffordshire, Keele, ST5 5BG, UK  
Journal of Inorganic Biochemistry (2001), 84(3-4), 215-224  
CODEN: JIBIDJ; ISSN: 0162-0134  
PUBLISHER: Elsevier Science Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The formation of amyloid fibrils is considered to be an important step in the etiol. of Alzheimer's disease and other amyloidoses. Fibril formation in vitro has been shown to depend on many different factors including modifications to the amino acid profile of fibrillogenic peptides and interactions with both large and small molecules of physiol. significance. How these factors might contribute to amyloid fibril formation in vivo is not clear as very little is known about the promotion of fibril formation in unresatd. solns. of amyloidogenic peptides. The authors have used thioflavin T fluorescence and reverse phase high performance liquid chromatog. to show that ATP, and in particular AlATP, promoted the formation of thioflavin T-reactive fibrils of  $\beta$  amyloid and, an unrelated amyloidogenic peptide, amylin. Evidence is presented that induction of fibril formation followed the complexation of AlATP by one or more monomers of the resp. peptide. However, the complex formed could not be identified directly and it is suggested that AlATP might be acting as a chaperone in the assembly of amyloid fibrils. The effect of AlATP was not mimicked by either AlADP or AlAMP. However, it was blocked by suramin, a p2 ATP receptor antagonist, and this has prompted us to speculate that the precursor proteins to  $\beta$  amyloid and amylin may be substrates or receptors for ATP in vivo.  
IT 2390-54-7, Thioflavin  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(amyloid fibrils formation promotion by aluminum ATP (AlATP))  
RN 2390-54-7 HCAPLUS  
CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 20 OF 388 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2001:186028 HCAPLUS Full-text  
DOCUMENT NUMBER: 134/233362  
TITLE: Minimal tau peptide for nucleation of paired helical filaments  
INVENTOR(S): Von Bergen, Martin; Biernat, Jacek; Mandelkow, Eva-Maria; Mandelkow, Eckhard  
PATENT ASSIGNER(S): Max-Planck-Gesellschaft Zur Foerderung Der Wissenschaften E.V., Germany; Von Bergen, Martin  
SOURCE: PCT Int. Appl., 91 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

10/511852 109/217 Robert Havlin

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001018546	A2	20010315	WO 2000-EP8863	20000911
WO 2001018546	A3	20010927		
WO 2001018546	A9	20020906		

M: AU, CA, JP, US  
RM: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

CA 2384006	A1	20010315	CA 2000-2384006	20000911
EP 1214598	A2	20020619	EP 2000-965965	20000911
EP 1214598	B1	20060517		

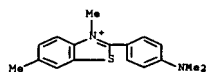
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY

JP 2003508788 T 20030304 JP 2001-522084 20000911  
AT 324700 T 20060615 AT 2000-965965 20000911  
EP 1999-117805 A 19990909  
WO 2000-EP8863 W 20000911

PRIORITY APPLN. INFO.:  
AB The present invention relates to a method for identifying and obtaining an inhibitor, capable of modifying the PHF (paired helical filaments) formation comprising the steps of (a) incubating a peptide comprising a specific tau derived peptide as defined herein or a fragment (a) thereof with a compound to be screened under conditions which permit assembly of said tau-derived peptides into nucleation sites for PHF assembly and/or into aggregation products; and (b) detecting the presence, decrease, or absence of nucleation sites for PHF assembly and/or the presence, decrease or absence of said aggregation products wherein said absence and/or decrease is indicative for putative inhibitors for PHF formation. Furthermore, the present invention provides inhibitors identified of obtained by said method as well as compns. comprising said inhibitor, wherein said composition is preferably a diagnostic and/or a pharmaceutical composition. The present invention further relates to a method for detecting and/or measuring PHF formation comprising the steps of (a) incubating a peptide comprising a specific tau derived peptide as defined herein or (a) fragment (a) thereof, with tau-proteins and/or fragments thereof under conditions which permit assembly of tau-proteins and/or fragments thereof into PHFs; and (b) detecting the presence, absence, decrease or increase of PHFs and/or nucleation sites of PHF assembly. The hexapeptide PHF6 (306-Val-Gln-Ile-Val-Tyr-Lys-311) of human tau23 represents a minimal interaction motif with a predicted  $\beta$ -structure conformation involved in PHF assembly. Addnl., the present invention provides for kits and uses for carrying out the method of the present invention.

IT 2390-54-7, Thioflavin T  
RI: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(assay of PHF formation; minimal tau peptide for nucleation of paired helical filaments)

RN 2390-54-7 HCAPLUS  
CN Benzothiazolium, 2-[4-(dimethylamino)phenyl]-3,6-dimethyl-, chloride (1:1)  
(CA INDEX NAME)



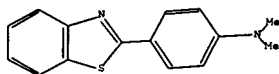
=>  
=> file reg

10/511852 111/217 Robert Havlin

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS 19:CLASS

L16 STRUCTURE UPLOADED

=> d  
L16 HAS NO ANSWERS  
L16 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l16 sss sam  
SAMPLE SEARCH INITIATED 14:41:32 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS 12 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 784 TO 1736  
PROJECTED ANSWERS: 33 TO 447

L17 12 SEA SSS SAM L16

=> s l16 sss full  
FULL SEARCH INITIATED 14:41:36 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1240 TO ITERATE

100.0% PROCESSED 1240 ITERATIONS 226 ANSWERS  
SEARCH TIME: 00.00.01

L18 226 SEA SSS PUL L16

=> d his

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L1 0 S 4992204/PN  
L2 0 S 4992204/PA  
L3 1 S US4992204/PN

FILE 'REGISTRY' ENTERED AT 14:28:06 ON 29 MAY 2007

FILE 'USPATFULL' ENTERED AT 14:28:12 ON 29 MAY 2007  
L4 TRA L3 1- RN : 74 TERMS

FILE 'REGISTRY' ENTERED AT 14:28:13 ON 29 MAY 2007

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	118.40	618.56

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL  
CA SUBSCRIBER PRICE -15.60 -34.32

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STRUCTURE FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2  
DICTIONARY FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

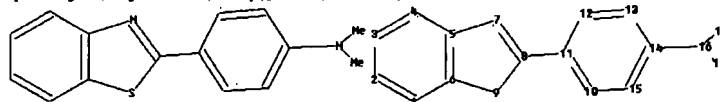
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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chain nodes :  
16 18 19  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15  
chain bonds :  
8-11 14-16 16-19  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15  
exact/norm bonds :  
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exact bonds :  
6-9 8-9 8-11 16-18 16-19  
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1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15  
isolated ring systems :  
containing 1 : 10

10/511852 112/217 Robert Havlin

L5	74 SEA L4
L6	STRUCTURE UPLOADED
L7	4 S L6 SSS SAM
L8	127 S L6 SSS FULL

FILE 'HCAPLUS' ENTERED AT 14:31:44 ON 29 MAY 2007  
24 S L8

FILE 'REGISTRY' ENTERED AT 14:32:19 ON 29 MAY 2007

L10 STRUCTURE UPLOADED  
L11 23 S L10 SSS SAM  
L12 437 S L10 SSS FULL  
L13 432 S L12 NOT L8

FILE 'HCAPLUS' ENTERED AT 14:38:26 ON 29 MAY 2007  
L14 568 S L13  
L15 388 S L14 AND PY <2002

FILE 'REGISTRY' ENTERED AT 14:41:13 ON 29 MAY 2007  
L16 STRUCTURE UPLOADED  
L17 12 S L16 SSS SAM  
L18 226 S L16 SSS FULL

=> s l13 not l18  
L19 206 L13 NOT L18

=> file hcaplus  
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL  
FULL ESTIMATED COST 172.10 790.66  
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL  
CA SUBSCRIBER PRICE 0.00 -34.32

FILE 'HCAPLUS' ENTERED AT 14:41:53 ON 29 MAY 2007  
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FILE COVERS 1907 - 29 May 2007 VOL 146 ISS 23  
FILE LAST UPDATED: 28 May 2007 (20070528/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L20 75 L19

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The search profile that was entered contains terms or  
nested terms that are not separated by a logical operator.

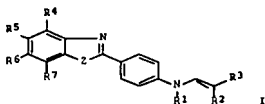
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4256240 PY > 2003  
L21 64 L20 NOT PY > 2003

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L21 ANSWER 1 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:673650 HCAPLUS Full-text  
DOCUMENT NUMBER: 139:218955  
TITLE: Synthesis of phenylamino derivatives of benzothiazole,  
benzoxazole and indazole for use as sunscreens  
INVENTOR(S): Dilk, Erich; Johncock, William; Langner, Roland  
PATENT ASSIGNEE(S): Haarmann & Reimer GmbH, Germany  
SOURCE: Ger. Offen., 30 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10206562	A1	20030828	DE 2002-10206562	20020218
PRIORITY APPLN. INFO.:			DE 2002-10206562	20020218
OTHER SOURCE(S):		MARPAT 139:218955		

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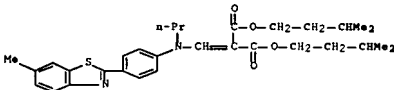


AB The invention concerns the synthesis of phenylamino deriva. of benzothiazole, benzoxazole and indazole with the general formula (I), where Z = NH, O or S; R groups are defined; the products are used as sunscreens. Other sunscreens can be added. Thus [[N-methyl-N-[4-(6-methyl-2-benzothiazol-2-yl)phenyl]amino]methylene]-propanedioic acid bis(2-ethylhexyl) ester was synthesized and included in a composition as a 3 weight/weight% ingredient; other components were (weight/weight%): Crodafor MCA 1.50; Cutina MD 2.00; Copherol 1250 0.50; Lanette 16 1.00; Tegosoft TN 24.00; Priosorine 3505 1.00; water 59.6; Tetrasodium EDTA 0.20; glycerin (99%) 3.00; phenoxyethanol 0.70; Solbrol M 0.20; Solbrol P 0.10; Carbopol ETD 2050 0.20; sodium hydroxide (10% aqueous solution) 2.70; perfume 0.30.

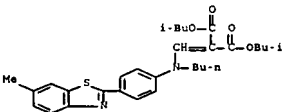
IT 586356-10-7P 586356-11-8P 586356-12-9P  
586356-13-OP 586356-14-1P 586356-16-3P  
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of phenylamino deriva. of benzothiazole and benzoxazole and indazole for use as sunscreens)

RN 586356-10-7 HCAPLUS  
CN Propanedioic acid, [[methyl[4-(6-methyl-2-benzothiazolyl)phenyl]amino]meth

RN 586356-14-1 HCAPLUS  
CN Propanedioic acid, [[4-(6-methyl-2-benzothiazolyl)phenyl]propylamino]meth ylene]-, bis(3-methylbutyl) ester (9CI) (CA INDEX NAME)



RN 586356-16-3 HCAPLUS  
CN Propanedioic acid, [[butyl[4-(6-methyl-2-benzothiazolyl)phenyl]amino]meth ylene]-, bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)

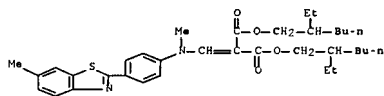


L21 ANSWER 2 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2002:539333 HCAPLUS Full-text  
DOCUMENT NUMBER: 137:116971  
TITLE: Photosensitive compositions for presensitized lithographic plates and their photopolymerization by laser scanning  
INVENTOR(S): Murota, Yasufumi; Sorori, Tadashi  
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.  
CODEN: JKKXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

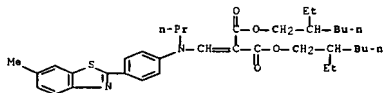
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002202596	A	20020719	JP 2000-401891	20000328
PRIORITY APPLN. INFO.:			JP 2000-401891	20000328
OTHER SOURCE(S):		MARPAT 137:116971		

AB The photosensitive compns. having high sensitivity to semiconductor laser light and good storage stability contain sensitizing dyes shown as (AaR1:N:R2).Z- (Ar = aromatic ring; A = NR3R4, SR5, OR6; R = H, monovalent nonmetal atom. group; Z = counter ion which may not be necessary when the dye cation part has anionic substituent; preferably, Z = halogen, perchlorate, tetrafluoroborate, hexafluorophosphate, (aryl)sulfonate), titanocenes, and

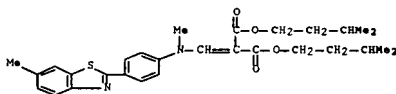
ylene]-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)



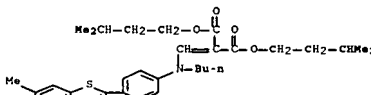
RN 586356-11-8 HCAPLUS  
CN Propanedioic acid, [[4-(6-methyl-2-benzothiazolyl)phenyl]propylamino]meth ylene]-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)



RN 586356-12-9 HCAPLUS  
CN Propanedioic acid, [[methyl[4-(6-methyl-2-benzothiazolyl)phenyl]amino]meth ylene]-, bis(3-methylbutyl) ester (9CI) (CA INDEX NAME)



RN 586356-13-0 HCAPLUS  
CN Propanedioic acid, [[butyl[4-(6-methyl-2-benzothiazolyl)phenyl]amino]meth ylene]-, bis(3-methylbutyl) ester (9CI) (CA INDEX NAME)

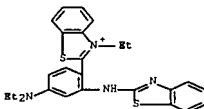


polymerizable compds. which may be addition-polymerizable compds. bearing ethylenically unsatd. double bonds. The compns. are polymerized by exposing to 5450-nm laser light.

IT 442874-09-1 442874-17-1  
RL: CAT (Catalyst use); USES (Uses)  
(sensitizing dye; photosensitive compns. for presensitized lithog. plates for semiconductor laser scanning)

RN 442874-09-1 HCAPLUS  
CN Benzothiazolium, 2-[2-(2-benzothiazolylamino)-4-(diethylamino)phenyl]-3-ethyl-, (T-4)-tetrachlorozincate(2-) (2:1) (9CI) (CA INDEX NAME)

CM 1  
CRN 88851-23-4  
CMP C26 H27 N4 S2

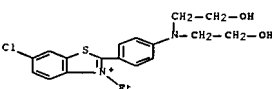


CM 2  
CRN 15201-05-5  
CMP C14 Zn  
CCI CCS



RN 442874-17-1 HCAPLUS  
CN Benzothiazolium, 2-[4-[bis(2-hydroxyethyl)amino]phenyl]-6-chloro-3-ethyl-, (T-4)-hexyltriphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1  
CRN 442874-16-0  
CMP C19 H22 Cl N2 O2 S

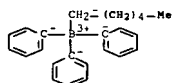


CM 2

CRN 131537-65-0

CMF C24 H28 B

CCI CCS



L21 ANSWER 3 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:792340 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 135:331672  
 TITLE: Preparation of methionine derivatives as inhibitors of protein isoprenyl transferases  
 INVENTOR(S): Sebt, Said M.; Hamilton, Andrew D.; Augeri, David J.; Barr, Kenneth J.; Fakhoury, Stephen A.; Janowick, David A.; Kalvin, Douglas M.; O'Connor, Stephen J.; Rosenberg, Saul H.; Shen, Wang; Swenson, Rolf E.; Sorenson, Bryan K.; Sullivan, Gerard M.; Tasker, Andrew S.; Wasicak, James T.; Nelson, Liisa T. J.; Henry, Kenneth J.; Wang, Le  
 PATENT ASSIGNER(S): University of Pittsburgh, USA  
 SOURCE: U.S., 514 pp., Cont.-in-part of U.S. Ser. No. 852,858, abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 8  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6310095	B1	20011030	US 1998-73794	19980507
EA 9906763	A	20000515	ZA 1999-6763	19991027
PRIORITY APPL. INFO.:			US 1995-72479	P 19951106
			US 1996-740909	B2 19961105
			US 1997-852858	B2 19970507
			US 1998-73794	A 19980507
			US 1998-197279	A 19981120

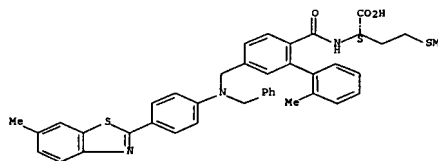
OTHER SOURCE(S): MARPAT 135:331672  
 AB Compds. R3-Z-L1-aryl [aryl is a benzene ring having certain substituents R1, R2, R4; L1 is LAMR515 where L4 and L5 are absent or alkylene, R5 is H, alkanoyl, alkoxy, alkoxyalkyl, haloalkyl, etc.; Z is a covalent bond; R3 = cycloalkyl, alkoxy, alkyl, halogen, oxo, etc.] or their pharmaceutically acceptable salts, were prepared as inhibitors of protein isoprenyl transferases. Thus, N-4-[(R)-thiazolidin-4-ylcarboxylamino]-2-phenylbenzoyl]methionine Me ester hydrochloride, prepared via amidation reaction, showed 94% inhibition of farnesyl transferase at 1x10<sup>-6</sup> M.  
 IT 216233-18-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of methionine derivs. as inhibitors of protein isoprenyl transferases)

RN 216233-18-0 HCAPLUS

CN L-Methionine, N-[[2'-methyl-5-[[[4-(6-methyl-2-benzothiazolyl)phenyl](phenylmethyl)amino]methyl][1,1'-biphenyl]-2-yl]carbonyl]-, monolithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

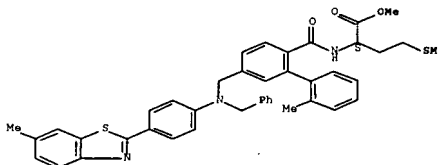


IT 216229-12-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of methionine derivs. as inhibitors of protein isoprenyl transferases)

RN 216229-12-1 HCAPLUS

CN L-Methionine, N-[[2'-methyl-5-[[[4-(6-methyl-2-benzothiazolyl)phenyl](phenylmethyl)amino]methyl][1,1'-biphenyl]-2-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 4 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:496097 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 133:278270  
 TITLE: New ratiometric fluorescent calcium indicators with moderately attenuated binding affinities

AUTHOR(S): Gee, K. R.; Archer, E. A.; Lapham, L. A.; Leonard, M.

CORPORATE SOURCE: S.; Zhou, Z.-L.; Bingham, J.; Divu, Z.

SOURCE: Molecular Probes, Inc., Eugene, OR, 97402, USA

Bioorganic &amp; Medicinal Chemistry Letters (2000),

10(14), 1515-1518

CODEN: BMLC88; ISSN: 0960-894X

Elsevier Science Ltd.

PUBLISHER: Journal

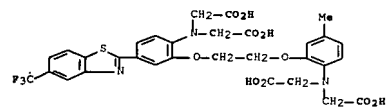
DOCUMENT TYPE: English

AB Mono-halogenated derivative of the calcium indicators fura-2 and indo-1 were synthesized and their spectroscopic properties evaluated. Halogenation ortho or para to the bridging oxygen in the BAPTA nucleus had a more pronounced weakening effect on binding affinity than in the meta position in the fura derivative. Two new excitation ratioable fluorescent calcium indicators, benzothiazole-1 and 2, were also synthesized. Kd values of 400 nM to 5.3 μM [Ca<sup>2+</sup>] were observed in these families of new probes.

IT 299172-12-6P 299172-26-2P  
 RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 (new ratiometric fluorescent calcium indicators with moderately attenuated binding affinities)

RN 299172-12-6 HCAPLUS

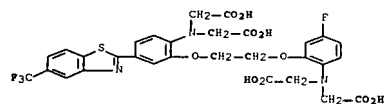
CN Glycine, N-[2-[2-[2-[bis(carboxymethyl)amino]-5-methylphenoxy]ethoxy]-4-[5-(trifluoromethyl)-2-benzothiazolyl]phenyl]-N-(carboxymethyl)-, tetrapotassium salt (9CI) (CA INDEX NAME)



● 4 K

RN 299172-26-2 HCAPLUS

CN Glycine, N-[2-[2-[2-[bis(carboxymethyl)amino]-5-fluorophenoxy]ethoxy]-4-[5-(trifluoromethyl)-2-benzothiazolyl]phenyl]-N-(carboxymethyl)-, tetrapotassium salt (9CI) (CA INDEX NAME)



● 4 K

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 5 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:567003 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:299398

TITLE: Antitumor benzothiazoles. 8. Synthesis, metabolic formation, and biological properties of the C- and N-oxidation products of antitumor 2-(4-aminophenyl)benzothiazoles

AUTHOR(S): Kaehiyama, Eiji; Hutchinson, Ian; Chua, Mei-Sze; Stinson, Sherman P.; Phillips, Lawrence R.; Kaur, Gurmeet; Sausville, Edward A.; Bradshaw, Tracey D.; Westwell, Andrew D.; Stevens, Malcolm P. G.  
 CORPORATE SOURCE: Pharmacology and Experimental Therapeutics Section, Laboratory of Drug Discovery Research and Development, Developmental Therapeutics Program, Division of Cancer Treatment and Diagnosis National Cancer Institute National Institutes of Health, Frederick, MD, 21702-1201, USA

SOURCE: Journal of Medicinal Chemistry (1999), 42(20), 4172-4184

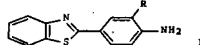
CODEN: JMCMAJ; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



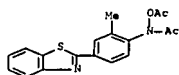
AB 2-(4-Aminophenyl)benzothiazoles I (R = Me, H, Cl, iodo, Br) and their N-acetylated forms have been converted to C- and N-hydroxylated derivs. to investigate the role of metabolic oxidation in the mode of action of this series of compds. 2-(4-Amino-3-methylphenyl)benzothiazole (II, DF 303, NSC 674495) is a novel and potent antitumor agent with selective growth inhibitory properties against human cancer cell lines. Very low IC50 values (<0.1 μM) were encountered in the most sensitive breast cancer cell lines, MCF-7 and T-47D, whereas renal cell line TK-10 was weakly inhibited by Ia. Cell lines from the same tissue origin, MDA-MB-435 (breast), CAKI-1 (renal), and A498 (renal), were insensitive to II. Accumulation and metabolism of Ia were observed in sensitive cell lines only, with the highest rate of metabolism occurring in the most sensitive MCF-7 and T-47D cells. Thus, differential uptake and metabolism of II by cancer cell lines may underlie its selective profile of anticancer activity. A major metabolite in these sensitive cell lines has been identified as 2-(4-amino-3-methylphenyl)-6-hydroxybenzothiazole (III). Hydroxylation of Ia was not detected in the homogenate of previously untreated MCF-7, T-47D, and TK-10 cells but was readily observed in homogenates of sensitive cells that were pretreated with II. Accumulation and covalent binding of [14C]Ia derived radioactivity was observed in the sensitive MCF-7 cell line but not in the insensitive MDA-MB-435 cell line. The mechanism of growth inhibition by II, which is unknown, may be dependent on the differential metabolism of the drug to an activated form by sensitive cell lines only and its covalent binding to an intracellular protein. However, the 6-hydroxy derivative III is not the 'active' metabolite since, like all other C- and N-hydroxylated benzothiazoles examined in this study, it is devoid of antitumor properties in vitro.

IT 247086-50-SP 247083-51-9P

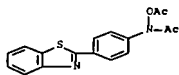
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, cytotoxicity, and antitumor activity of

RN 247080-50-8 HCAPLUS  
CN Acetamide, N-(acetyloxy)-N-[4-(2-benzothiazolyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)

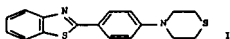


RN 247080-51-9 HCAPLUS  
CN Acetamide, N-(acetyloxy)-N-[4-(2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)

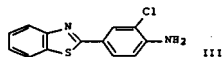
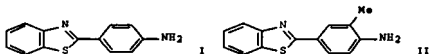


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 6 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1999:333877 HCAPLUS Full-text  
DOCUMENT NUMBER: 131:170336  
TITLE: Synthesis and silver ion complexation behavior of fluoroionophores containing a benzothiazolyl group linked to an N-phenylpolythiazalkane moiety  
AUTHOR(S): Ishikawa, Junichi; Sakamoto, Hidefumi; Wada, Hiroko  
CORPORATE SOURCE: Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466-8555, Japan  
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1999), (6), 1273-1280  
CODEN: JCPKDH; ISSN: 0300-9580  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OI



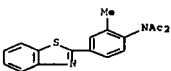
AB Cyclic and acyclic polythiazalkane derive., e.g., I, bearing a benzothiazolyl group as a fluorophore have been synthesized. The protonation and the metal ion complexation behavior were studied in a 1,4-dioxane-water (52/48 volume/volume) solution by spectrophotometry and/or spectrofluorometry. The changes in the absorption spectra (blue



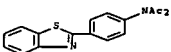
AB 2-(4-Aminophenyl)benzothiazoles display potent and selective antitumor activity against inter alia breast, ovarian, colon, and renal cell lines, but their mechanism of action, though yet to be defined, may be novel. Metabolism is suspected to play a central role in the mode of action of these benzothiazoles since drug uptake and biotransformation were observed in sensitive cell lines (e.g., breast MCF-7 and MDA 468 cells) in vitro, whereas insensitive cell lines (e.g., prostate PC 3 cells) showed negligible uptake and biotransformation. N-Acyl derivative of the arylamines have been synthesized, and in vitro studies confirm N-acetylation and oxidation as the main metabolic transformations of 2-(4-aminophenyl)benzothiazoles, with the predominant process being dictated by the nature of the 3'-substituent. The prototype amine I underwent mainly N-acetylation in vitro, while 3'-substituted analogs II and III were primarily oxidized. N-Acetylation exerts a drastic dyshemotherapeutic effect in vitro, but acetylation of halogeno congeners gave acetylamines which substantially retain selective antitumor activity. In vivo pharmacokinetic studies in rats confirmed rapid and exclusive N-acetylation of the 3'-Me analog II, but less acetylation with the 3'-chloro analog III. Distinct expression patterns of N-acetyltransferase NAT1 and NAT2 have been demonstrated in our panel of cell lines.

IT 182274-77-7P 220222-20-0P 220222-21-3P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(acetylamino)benzothiazole preparation and role of acetylation in antitumor activities of parent amines)

RN 182274-77-7 HCAPLUS  
CN Acetamide, N-acetyl-N-[4-(2-benzothiazolyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)

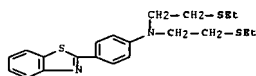


RN 220222-20-0 HCAPLUS  
CN Acetamide, N-acetyl-N-[4-(2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)

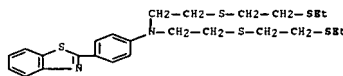


shift and hypochromic effect) and the fluorescence emission spectra (quenching) were observed by the addition of Ag<sup>+</sup> ion selectively. On complexation with the Ag<sup>+</sup> ion, the degree of the spectral changes of the benzothiazole derivative, is dependent on the extent of the interactions of the complexed Ag<sup>+</sup> ion with the nitrogen atom of the polythiazalkane moiety and with the benzothiazolylphenyl moiety. The complexation and the protonation behavior of the benzothiazole derivative were investigated using <sup>1</sup>H NMR spectroscopy.

IT 239103-02-2P 239103-03-3P  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation; complexation, and fluorescence of benzothiazolyl phenylpolythiazalkanes)  
RN 239103-02-2 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-bis[2-(ethylthio)ethyl]- (9CI) (CA INDEX NAME)



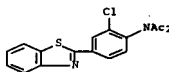
RN 239103-03-3 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-bis[2-(ethylthio)ethyl]thioethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 7 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1999:59397 HCAPLUS Full-text  
DOCUMENT NUMBER: 130:261585  
TITLE: Antitumor Benzothiazoles. 7. Synthesis of 2-(4-Acylaminophenyl)benzothiazoles and Investigations into the Role of Acetylation in the Antitumor Activities of the Parent Amines  
AUTHOR(S): Chua, Mei-Sze; Shi, Dong-Pang; Wrigley, Samantha; Bradshaw, Tracey D.; Hutchinson, Ian; Shaw, P. Nicholas; Barrett, David A.; Stanley, Lesley A.; Stevens, Malcolm F. G.  
CORPORATE SOURCE: Cancer Research Laboratories, School of Pharmaceutical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Journal of Medicinal Chemistry (1999), 42(3), 381-392  
CODEN: JMCMAH; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OI

RN 220222-21-1 HCAPLUS  
CN Acetamide, N-acetyl-N-[4-(2-benzothiazolyl)-2-chlorophenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 8 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1998:744940 HCAPLUS Full-text  
DOCUMENT NUMBER: 130:25338  
TITLE: Inhibitors of protein isoprenyl transferases  
INVENTOR(S): Sebti, Said M.; Hamilton, Andrew D.; Augeri, David J.; Barr, Kenneth J.; Donner, Bernard G.; Fakhoury, Stephen A.; Janowick, David A.; Kalvin, Douglas M.; Larsen, John J.; Liu, Gang; O'Connor, Stephen J.; Rosenberg, Saul H.; Shen, Wang; Swenson, Rolf E.; Sorensen, Bryan K.; Sullivan, Gerard M.; Szczepankiewicz, Bruce G.; Tasker, Andrew S.; Wasick, James I.; Winn, Martin  
PATENT ASSIGNER(S): University of Pittsburgh, USA  
SOURCE: PCT Int. Appl., 848 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 8  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9850029	A1	19981112	WO 1998-09296	19980507
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, ES, SE, FI, GB, GE, GR, HU, IL, IS, JP, KR, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RN: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CP, CO, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2288330	A1	19981112	CA 1998-2288330	19980507
AU 9874733	A	19981127	AU 1998-74733	19980507
EP 986384	A1	20000322	EP 1998-922122	19980507
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002518985	T	20020625	JP 1998-546480	19980507
TW 492955	B	20020701	TW 1998-07107182	19980715
TW 541302	B	20030711	TW 1998-07107183	19980715
MX 9910186	A	20000630	MX 1999-10186	19991105
PRIORITY APPL. INFO.:				
US 1997-852858	A	19970507	WO 1998-US9296	19980507
OTHER SOURCE(S):			MARPAT 130:25338	

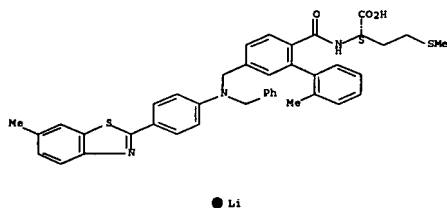
10/511852 125/217 Robert Havlin

AB Compds. R3-2-L1-aryl [aryl is a benzene ring having certain substituents R1, R2, R4; L1 is absent or is L4NR5L5, L4OL5, L4S(O)MeL5 (m = 0-2), etc., where L4 and L5 are absent or alkylene, alkenylene, R5 is H, alkenyl; Z is a covalent bond, O, S(O)q (q = 0-2), NH or imino; R3 = H, aryl, fluorenyl, heterocyclyl, cycloalkyl, etc.] were prepared as inhibitors of protein isoprenyl transferases. Thus, N-[4-[(R)-thiazolidin-4-ylcarbonylamino]-2-phenylbenzoyl]methionine Me-ester hydrochloride, prepared via amidation reaction, showed 92% inhibition of farnesyl transferase at 1x10<sup>-6</sup> M.

IT 216233-18-0P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PRPP (Preparation); USES (Uses)  
[preparation of inhibitors of protein isoprenyl transferases]

RN 216233-18-0 HCAPLUS  
CN L-Methionine, N-[[2'-methyl-5-[[[4-(6-methyl-2-benzothiazolyl)phenyl](phenylmethyl)amino]methyl][1,1'-biphenyl]-2-yl]carbonyl]-, monolithium salt (9CI) (CA INDEX NAME)

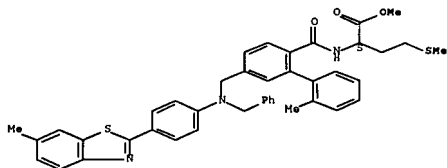
Absolute stereochemistry.



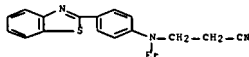
IT 216229-23-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
[preparation of inhibitors of protein isoprenyl transferases]

RN 216229-23-1 HCAPLUS  
CN L-Methionine, N-[[2'-methyl-5-[[[4-(6-methyl-2-benzothiazolyl)phenyl](phenylmethyl)amino]methyl][1,1'-biphenyl]-2-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

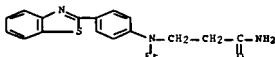
Absolute stereochemistry.



10/511852 127/217 Robert Havlin



RN 127868-59-1 HCAPLUS  
CN Propanamide, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 10 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1996:717765 HCAPLUS Full-text  
DOCUMENT NUMBER: 126:74784  
TITLE: Synthesis and biological evaluation of new allylamine antimycotics  
AUTHOR(S): Chung, Byung-Ho; Park, Eun-Ju; Moon, Hyun-Ju; Yoo, Jin-Cheol  
CORPORATE SOURCE: College Pharmacy, Chonnam National University, Kwang Ju, 500-757, S. Korea  
SOURCE: Yakshak Boechi (1996), 40(5), 507-512  
CODEN: YAKHQA; ISSN: 0511-4234  
PUBLISHER: Pharmaceutical Society of Korea  
DOCUMENT TYPE: Journal  
LANGUAGE: Korean

AB Benzothiazolyl-substituted allylamines were prepared as potential antimycotics. Thus, intermediate Schiff bases, obtained by condensation of 2-aminobenzothiazoles and trans-cinnamaldehyde, were reduced and then methylated to give the benzothiazolyl-substituted allylamines. These compds., which were tested in vitro against five fungal cell lines containing Trichophyton mentagrophytes, showed no activity in the 0.1-100 µg/mL range.

IT 185430-88-0P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
[preparation and fungicidal activity of benzothiazolyl-substituted allylamines]

RN 185430-88-0 HCAPLUS  
CN Benzenamine, N-methyl-4-(6-methyl-2-benzothiazolyl)-N-(3-phenyl-2-propenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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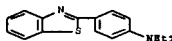
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 9 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1997:787209 HCAPLUS Full-text  
DOCUMENT NUMBER: 128:88508  
TITLE: Effect of the medium acidity on the photophysical characteristics of some 2-aryl- and 2-hetarylbenzothiazoles  
AUTHOR(S): Petkov, I.; Deligeorgiev, T.; Timcheva, I.  
CORPORATE SOURCE: Faculty of Chemistry, University of Sofia, Sofia, 1164, Bulg.  
SOURCE: Dyes and Pigments (1997), 35(2), 171-181  
CODEN: DYPIDX; ISSN: 0143-7208  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

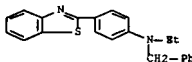
AB The absorption and fluorescence spectral characteristics of 2-aryl- and 2-hetarylbenzothiazoles and their protonated forms in solution were studied. The influence of structural modifications on the position of their absorption and fluorescence maxima, as well as interesting features with respect to competition in protonation between the benzothiazole and aniline or hetaryl nitrogen atom in the ground (S0) state has been studied. The influence of pH on the absorption and the emission spectra of all the compds. has been investigated in order to identify the ground state species present as a function of acidity.

IT 10205-57-9 55489-36-6 127868-58-0  
127868-59-1  
RL: PRP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(medium acidity effect on photophys. characteristics of aryl- and hetarylbenzothiazoles)

RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

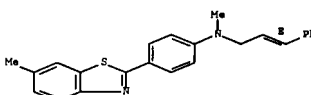


RN 55489-36-6 HCAPLUS  
CN Propanethanamine, N-[[4-(2-benzothiazolyl)phenyl]N-ethyl]- (9CI) (CA INDEX NAME)



RN 127868-58-0 HCAPLUS  
CN Propanenitrile, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)

10/511852 128/217 Robert Havlin



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L21 ANSWER 11 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1995:835470 HCAPLUS Full-text  
DOCUMENT NUMBER: 123:228181  
TITLE: Preparation of imidazolylalkylamine derivatives as steroid 17-20 lyase inhibitors  
INVENTOR(S): Okada, Minoru; Yoden, Toru; Kawaminami, Eiji; Shimada, Yoshiaki; Ishihara, Teikase; Kudou, Masafumi  
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 165 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9504723	A1	19950216	WO 1994-JP1278	19940803
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KE, KR, KZ, LK, LT, LV, MD, MG, MN, MM, NO, NZ, PL, PT, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ, VN				
RM: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CP, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9472758	A	19950228	AU 1994-72758	19940803
PRIORITY APPLN. INFO.:			JP 1993-193635	A 19930804
OTHER SOURCE(S):			WO 1994-JP1278	W 19940803
GI			MARPAT 123:228181	



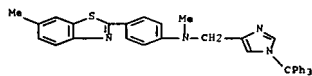
AB Title compds. I [R1 = H, alkyl; A1 = optionally branched lower alkylene; A2 = optionally bonded or branched lower alkylene; R2 = (un)substituted Ph, (un)substituted bi- or tricyclic hydrocarbon ring having fused benzene ring(s), (un)substituted bi- or tricyclic fused hetero ring having fused benzene ring(s) and a hetero ring containing oxygen and/or sulfur and/or nitrogen as the hetero atom(s); R3 = alkyl, lower alkenyl, lower alkynyl, cycloalkyl, A3R4, halogen-substituted lower alkyl, cyano-substituted lower alkyl, (un)substituted hetero ring containing nitrogen as the hetero atom(s); A3 = optionally branched lower alkylene or carbonyl; R4 = (un)substituted cycloalkyl, (un)substituted Ph, or (un)substituted hetero ring containing nitrogen as the hetero atom(s)] and their

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pharmaceutically acceptable salts, useful as steroid 17-20 lyase inhibitors, were prepared. Thus, reaction of 6-[N-(1-trityl-1H-imidazol-4-ylmethyl)amino]-2-methylbenzothiazole with p-chlorobenzyl bromide and NaH in DMF gave, after deprotection with 1N HCl, 6-[N-(3-chlorobenzyl)-N-(1H-imidazol-4-ylmethyl)amino]-2-methylbenzothiazole. 4-[[N-ethyl-N-(9H-fluoren-2-yl)amino]methyl]-1H-imidazole had an IC50 of 5.5 nM against steroid 17-20 lyase.

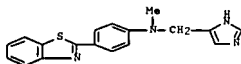
IT 168631-44-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of imidazolylalkylamine deriva. as steroid 17-20 lyase inhibitors)

RN 168631-44-5 HCAPLUS  
 CN 1H-imidazole-4-methanamine, N-methyl-N-[4-(6-methyl-2-benzothiazolyl)phenyl]-1-(triphenylmethyl)- (9CI) (CA INDEX NAME)



IT 168630-65-7P  
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of imidazolylalkylamine deriva. as steroid 17-20 lyase inhibitors)

RN 168630-65-7 HCAPLUS  
 CN 1H-imidazole-4-methanamine, N-[4-(2-benzothiazolyl)phenyl]-N-methyl- (9CI) (CA INDEX NAME)



L21 ANSWER 12 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1995:495508 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 122:230770  
 TITLE: Benzazole compounds for use in therapy  
 INVENTOR(S): Stevens, Malcolm Francis Graham; McCall, Carol Jane; Lelieveld, Petrus  
 PATENT ASSIGNEE(S): Cancer Research Campaign Technology Ltd., UK  
 SOURCE: PCT Int. Appl., 47 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9506469	A1	19950309	WO 1994-GB1883	19940830
M: AU, CA, JP, US				

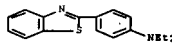
10/511852 130/217 Robert Havlin

RM: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
 CA 2170508 A1 19950309 CA 1994-2170508 19940830  
 AU 9475049 A 19950322 AU 1994-75049 19940830  
 AU 690577 B2 19980430  
 EP 721336 A1 19960717 EP 1994-924946 19940830  
 SP 721336 B1 19990714  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE  
 JP 09501944 T 19970225 JP 1994-508001 19940830  
 AT 182077 T 19990715 AT 1994-924946 19940830  
 ES 2133571 T 19990916 ES 1994-924946 19940830  
 US 5874431 A 19990223 US 1996-615845 19960228  
 GR 3031418 T3 20000131 GR 1999-402507 19991007  
 GB 1993-17949 A 19930828  
 WO 1994-GB1883 W 19940830

PRIORITY APPLN. INFO.:  
 OTHER SOURCE(S): CASREACT 122:230770; MARPAT 122:230770  
 AB There are disclosed herein benzazole compds., exemplified by 2-(4-aminophenyl)benzothiazole (I) and analogs or salts thereof, which exhibit very significant selective cytotoxic activity in respect of tumor cells, especially breast cancer cells, and which provide potentially useful chemotherapeutic agents for treatment of breast cancer. I was prepared from 2-aminothiophenol and 4-aminobenzoic acid. I showed a high and selective activity as an antiproliferative agent in cultures of MCF-7 mammary carcinoma cells.

IT 10205-57-9  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (preparation of benzothiazoles for treatment of breast cancer)

RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 13 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1995:80816 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 122:203999  
 TITLE: Study on the micellar color reaction of nickel with 2-(2-thiazolylazo)-5-diethylaminobenzoic acid  
 AUTHOR(S): Chen, Zhanguang; Chen, Tongsen; Zheng, En  
 CORPORATE SOURCE: Peop. Rep. China  
 SOURCE: Yejin Fenxi (1993), 13(5), 14-17  
 CODEN: YEFRET; ISSN: 1000-7571

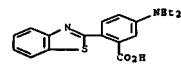
DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese

AB The micellar color reaction of nickel with 2-(2-thiazolylazo)-5-diethylaminobenzoic acid (TABS) in the presence of Tween-80 and its application to spectrophotometric determination of trace nickel were studied. In the pH range of 4.8-5.7 nickel formed a stable complex with TABS and the apparent molar absorptivity was 1.43 x 105 at 614 nm. The molar ratio of nickel to TABS is 1:1. Beer's law was obeyed at 0-6.0 µg/10 mL for nickel. The method was applied to the determination of trace nickel in aluminum alloys and no prior separation was required.

IT 161822-31-7  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (determination of nickel by spectrophotometry with 2-(2-thiazolylazo)-5-diethylaminobenzoic acid)

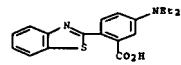
RN 161822-31-7 HCAPLUS  
 CN Benzoic acid, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)

10/511852 131/217 Robert Havlin



IT 161822-31-7D, nickel complex  
 RL: PREP (Preparation)  
 (visible spectrum of)

RN 161822-31-7 HCAPLUS  
 CN Benzoic acid, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



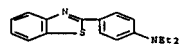
L21 ANSWER 14 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1995:22848 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 122:92540  
 TITLE: a new pseudophotochromic benzothiazoles doped PVC films  
 AUTHOR(S): Petkov, Ivan; Deligeorgiev, Todor; Sertova, Nadejda  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. Sofia, Sofia, 1126, Bulg.  
 SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1994), 246, 359-65  
 CODEN: MCLCE9; ISSN: 1058-725X

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Under the influence of the UV light in 2-aryl substituted benzothiazoles doped PVC films take shapes a new pseudophotochromic system. The colored films were formed by two processes: the liberation of HCl during the photodegradn. of PVC and an interaction between HCl and 2-arylsubstituted benzothiazoles (BT). They can return thermally to the colorless films and this process depends on the stability of the complexes BTn.Cl-. Reversible photochromism was observed in the films on repeating irradiation with UV light. The expl. results, possible applications and future work on this pseudophotochromic system are also discussed.

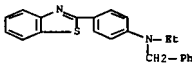
IT 10205-57-9 55469-36-6 127868-58-0  
 127868-59-1  
 RL: MCA (Modifier or additive use); PREP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 (photochromism of benzothiazoles doped PVC films)

RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

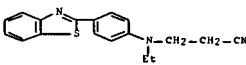


10/511852 132/217 Robert Havlin

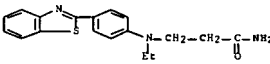
RN 55469-36-6 HCAPLUS  
 CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-ethyl- (9CI) (CA INDEX NAME)



RN 127868-58-0 HCAPLUS  
 CN Propanenitrile, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)



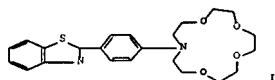
RN 127868-59-1 HCAPLUS  
 CN Propanamide, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)



L21 ANSWER 15 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1994:523962 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 121:123962  
 TITLE: Synthesis and spectral properties of a new benzothiazolic chromofluorophore containing the aza-15-crown-5 macrocyclic moiety  
 AUTHOR(S): Mateeva, N.; Deligeorgiev, T.; Mitewa, M.; Simova, S.; Dimov, I.  
 CORPORATE SOURCE: Dep. Chem., Univ. Sofia, Sofia, Bulg.  
 SOURCE: Journal of Inclusion Phenomena and Molecular Recognition in Chemistry (1994), 17(1), 81-91  
 CODEN: JIMCEH; ISSN: 0923-0750

DOCUMENT TYPE: Journal  
 LANGUAGE: English

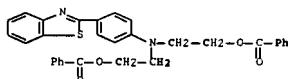




AB The synthesis of 1 [1-[(4-benzothiazolyl)phenyl]-4,7,10,13-tetraoxa-1-azacyclopentadecane], a new chromofluorophore is described. Its interaction with alkali and alkaline-earth metal salts in MeCN is studied both spectrophotometrically and spectrofluorometrically.

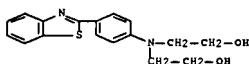
IT 156877-95-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and deprotection of)

RN 156877-95-1 HCAPLUS  
CN Ethanol, 2,2'-[[4-(2-benzothiazolyl)phenyl]imino]bis-, dibenzoate (ester) (9CI) (CA INDEX NAME)



IT 156877-96-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and methylation and cyclization reaction of, with triethylene glycol tosylate)

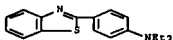
RN 156877-96-2 HCAPLUS  
CN Ethanol, 2,2'-[[4-(2-benzothiazolyl)phenyl]imino]bis- (9CI) (CA INDEX NAME)



IT 156877-92-8P 156877-93-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

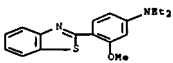
RN 156877-92-8 HCAPLUS  
CN Ethanol, 2-[[4-(2-benzothiazolyl)phenyl] (2-methoxyethyl)amino]- (9CI) (CA INDEX NAME)

CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



IT 149977-31-1P  
RL: PREP (Preparation)  
(laser and electronic spectra and synthesis of)

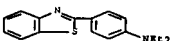
RN 149977-31-1 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl-3-methoxy- (9CI) (CA INDEX NAME)



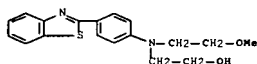
L21 ANSWER 17 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1994:190909 HCAPLUS Full-text  
DOCUMENT NUMBER: 120:190909  
TITLE: A comparative study. The photophysics of 2-phenylbenzothiazoles and 2-phenylbenzoxazoles  
AUTHOR(S): Chou, Pi-Tai; Cooper, William C.; Clements, John H.; Studer, Shannon L.; Chang, Chen Pin  
CORPORATE SOURCE: Department of Chemistry, University of South Carolina, Columbia, SC, 29208, USA  
SOURCE: Chemical Physics Letters (1993), 216(3-6), 300-4  
CODEN: CHPLBC; ISSN: 0009-2614  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The photophysics properties of the title compds. were compared. At room temperature 2-phenylbenzothiazole in n-heptane exhibits a broad, structureless absorption and a low fluorescence yield of 0.005 (if 200 ps). In contrast, 2-phenylbenzoxazole shows a structured absorption and a high fluorescence yield. These spectral differences arise from a drastic change in the dynamics of C1-C1' torsional motion, as evidenced in the temperature-dependent studies, spectral properties of their derivs. and AM1 calcs.

IT 10205-57-9  
RL: PRP (Properties)  
(fluorescence and UV spectra)

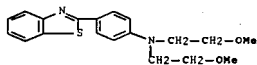
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 18 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1993:562363 HCAPLUS Full-text



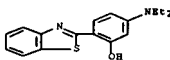
RN 156877-93-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-bis(2-methoxyethyl)- (9CI) (CA INDEX NAME)



L21 ANSWER 16 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1994:521097 HCAPLUS Full-text  
DOCUMENT NUMBER: 121:121097  
TITLE: Photophysics of 2-(4'-dialkylaminophenyl)benzothiazoles: their application for near-UV laser dyes  
AUTHOR(S): Chou, Pi Tai; Martinez, Marty L.; Cooper, William C.; Chang, Chen Pin  
CORPORATE SOURCE: Dep. Chem., Univ. South Carolina, Columbia, SC, 29208, USA  
SOURCE: Applied Spectroscopy (1994), 48(5), 604-6  
CODEN: APSPA4; ISSN: 0003-7028  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The photophysics, properties and the 1st observation of UV laser generation of mols. based on 2-phenylbenzothiazole with electron-donating substituents at the 2' and 4' positions are reported. The high gain of the amplified spontaneous emission, good efficient laser output, and extreme photostability for this class of laser dyes make their practical application feasible when pumped by the 3rd harmonic (355 nm) of the YAG laser.

IT 55489-32-2, 2-(2'-Hydroxy-4'-diethylaminophenyl)benzothiazole  
RL: USES (Uses)  
(dimethylsulfate reaction with, diethylaminophenylbenzothiazole laser dye synthesis by)

RN 55489-32-2 HCAPLUS  
CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



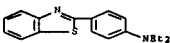
IT 10205-57-9, 2-(4'-Diethylaminophenyl)benzothiazole  
RL: USES (Uses)  
(laser and electronic spectra and photostability of)

RN 10205-57-9 HCAPLUS

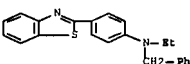
DOCUMENT NUMBER: 119:162363  
TITLE: Absorption and fluorescence characteristics of some 2-aryl- and 2-hetaryl-benzothiazoles  
AUTHOR(S): Timcheva, I.; Deligeorgiev, T.  
CORPORATE SOURCE: Cent. Phytochem., Inst. Org. Chem., Sofia, 1113, Bulg.  
SOURCE: Dyes and Pigments (1993), 21(4), 293-9  
CODEN: DYPIDX; ISSN: 0143-7208  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The absorption and fluorescence characteristics of some 2-aryl- and 2-hetarylbenzothiazoles were studied with respect to the nature of the substituents and the polarity of the solvents. The longest wavelength absorption maximum of these compds. is in the region 27,000-34,000 cm<sup>-1</sup>. The PPP-SCF-CI quantum chemical calcs. show that they result from a singlet  $\pi-\pi^*$  transition. The fluorescence Franck-Condon transition is between 19,000 and 28,000 cm<sup>-1</sup>. The fluorescence quantum yield of most of the investigated benzothiazoles exceeds 0.5. The compds. do not phosphoresce in frozen EtOH solns. at 77 K.

IT 10205-57-9 55489-36-6 127868-58-0  
127868-59-1  
RL: PRP (Properties)  
(absorption spectra and fluorescence of)

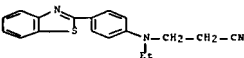
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



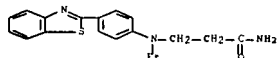
RN 55489-36-6 HCAPLUS  
CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-ethyl- (9CI) (CA INDEX NAME)



RN 127868-58-0 HCAPLUS  
CN Propanenitrile, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)

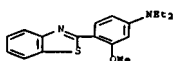


RN 127868-59-1 HCAPLUS  
CN Propanamide, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)

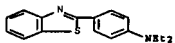


L21 ANSWER 19 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1993:559543 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 119:159543  
TITLE: Reinvestigation of the photophysics of  
2-(2'-hydroxy-4'-(diethylaminophenyl)benzothiazole  
AUTHOR(S): Chou, Pi Tai; Martinez, Marty L.  
CORPORATE SOURCE: Dep. Chem., Univ. South Carolina, Columbia, SC, 29208,  
USA  
SOURCE: Photochemistry and Photobiology (1993), 57(4), 593-6  
CODEN: PHCBAP; ISSN: 0031-8655  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The photophysics, properties of 2-(2'-hydroxy-4'-(diethylaminophenyl)benzothiazole (HABT)  
have been investigated by steady-state and time-resolved spectroscopies. In n-heptane  
HABT exhibits both normal and tautomer emissions with approx. equal fluorescence intensity  
at room temperature, in contrast to a previous report in which negligible tautomer  
emission was observed. The normal/tautomer (400/500 nm) ratio of emission intensity  
increases as the temperature decreases. Two possible excited-state intramol. proton  
transfer (ESIPT) mechanisms are proposed, which cannot be resolved at the present stage.  
One proposed mechanism incorporates state mixing between -OH and -N(C2H5)2 charge transfer  
states, resulting in a significant energy barrier for ESIPT. An alternative mechanism is  
also proposed in which fast proton tunneling may take place between enol and keto forms,  
which are in equilibrium in the excited singlet state.

IT 149977-31-1  
RL: PRP (Properties)  
(adsorption and emission spectra of)  
RN 149977-31-1 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl-3-methoxy- (9CI) (CA INDEX  
NAME)



IT 10205-57-9  
RL: PRP (Properties)  
(fluorescence of)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



TITLE: Luminescent compounds for the identification of  
materials by irradiation  
INVENTOR(S): Kluger, Edward W.; Moore, Patrick D.; Hines, John B.;  
Lever, John G.  
PATENT ASSIGNOR(S): Milliken Research Corp., USA  
SOURCE: U.S., 74 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

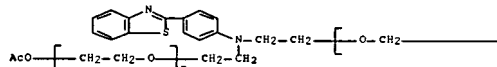
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4992204	A	19910212	US 1989-397079	19890822

PRIORITY APPLN. INFO.:  
US 1989-397079 19890822

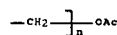
AB Synthetic or natural materials (e.g. silicone foams, dyed yarns) are detected or  
identified by tagging them with compds. of specified structure which absorb UV radiation  
at 300-400 nm and re-emit visible light. Polyoxyethylation of 183 g PhN(CH2CH2OH)2 with  
4400 g ethylene oxide, acetylation, and reaction with 306.8 g POCl3, 202.5 g DMF, and 20.4  
g Ac2O gave p-OCH2CH2NH[CH2CH2O]50Ac)2 (I). Heating I 166S, 2-H2NC6H4SH 37.6, and AcOH  
123 g at 190-200° for 4 h with distillation of AcOH gave a benzothiazole derivative of I  
with UV absorption maximum 362 nm, which emitted blue fluorescence. Use of this compound  
to identify dyed wool is described.

IT 134900-34-8P 135375-02-9P  
RL: IMP (Industrial manufacture); PRP (Properties); PREP (Preparation)  
(manufacture of, as fluorescent tags for identification of materials by  
irradiation)  
RN 134900-34-8 HCAPLUS  
CN Poly(oxy-1,2-ethanediyl),  $\alpha,\alpha'$ -[[[4-(2-  
benzothiazolyl)phenyl]imino]di-2,1-ethanediyl]bis[ $\alpha$ -(acetyloxy)-  
(9CI) (CA INDEX NAME)

PAGE 1-A

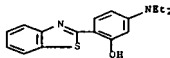


PAGE 1-B



RN 135375-02-9 HCAPLUS  
CN Oxirane, methyl-, polymer with oxirane, ether with 2,2'-[[[4-(6-methyl-2-  
benzothiazolyl)phenyl]imino]bis[ethanol] (2:1), block (9CI) (CA INDEX  
NAME)  
CM 1  
CRN 178667-44-2

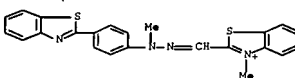
IT 55489-32-2  
RL: PRP (Properties)  
(keto-enol tautomerism of, fluorescence spectra in relation to)  
RN 55489-32-2 HCAPLUS  
CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



L21 ANSWER 20 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1993:170978 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 118:170978  
TITLE: Molecular structure of cationic dyes and their mixing  
properties  
AUTHOR(S): Xie, Kongliang; Yang, Jinzong; Hou, Yufen  
CORPORATE SOURCE: Inst. Chem. Eng., Dalian Univ. Technol., Dalian,  
116012, Peop. Rep. China  
SOURCE: Huangong Xuebao (Chinese Edition) (1992), 43(2), 247-54  
CODEN: HUKHAI; ISSN: 0438-1157  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese

AB The mixing properties of F-containing triazine and azo cationic dyes could be described by  
the inorg. value (I)-organic value (O) ratio of the dye. The organic and inorg. values of  
the dye could be as: O value =  $n \cdot 20 + \sum O_i$  and I value =  $\sum I_i$  (where n is the carbon nos.,  
O<sub>i</sub> and I<sub>i</sub> the organic value and inorg. value of the substitution group, resp.).

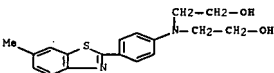
IT 146672-23-3  
RL: MSC (Miscellaneous)  
(dyes, mixing properties of, inorg. value-organic value ratio in relation  
to)  
RN 146672-23-3 HCAPLUS  
CN Benzothiazolium, 2-[[[4-(2-benzothiazolyl)phenyl]methylhydrazono]methyl]-3-  
methyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

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L21 ANSWER 21 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1991:494032 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 115:94032

CMF C18 H20 N2 O2 S



CM 2  
CRN 106392-12-5  
CMF (C3 H6 O . C2 H4 O)x  
CCI PMS  
CM 3  
CRN 75-56-9  
CMF C3 H6 O



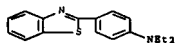
CM 4  
CRN 75-21-8  
CMF C2 H4 O



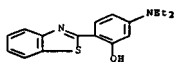
L21 ANSWER 22 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1991:111679 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 114:111679  
TITLE: New features in the photophysics and photochemistry of  
2-(2'-hydroxyphenyl)benzothiazoles introduced by amine  
substitution  
AUTHOR(S): Lenoble, Christian; Becker, Ralph S.  
CORPORATE SOURCE: Dep. Chem., Univ. Houston, Houston, TX, 77204, USA  
SOURCE: Photochemistry and Photobiology (1990), 52(6), 1063-9  
CODEN: PHCBAP; ISSN: 0031-8655  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The photophysics and photochem. of the 4'-(diethylamino derivative of both 2-  
phenylbenzothiazole and 2-(2'-hydroxyphenyl)benzothiazole were studied by nanosecond and  
microsecond laser flash photolysis and picosecond emission spectroscopy. For the non-  
hydroxy substituted mol., the singlet excited state relaxed primarily via fluorescence  
emission, and a very weak triplet transient was observed after laser flash excitation.

The 2-(2'-hydroxy-4'-diethylaminophenyl)benzothiazole (AHBT) underwent excited state intramol. proton transfer (ESIPT) in the picosecond timescale ( $k > 3 \times 10^{10} \text{ s}^{-1}$ ) to form a colored zwitterion/keto form in solution at room temperature whereas the ground state back proton transfer was slower by a factor of approx.105. However, in marked contrast with other derivs. of 2-(2'-hydroxyphenyl)benzothiazole and related mols., the ESIPT was not the only deactivation process of the lowest singlet excited state of the enol form. Under steady-state excitation at room temperature (and low temperature), the fluorescence emission of the enol form was observed. The T-T absorption of the enol form was also observed and furthermore, the ESIPT had an activation energy which was estimated to be approx.4 kJ. None of the foregoing, fluorescence and T-T absorption of the enol nor activation energy for proton transfer were observed for the parent or derivs. of 2-(2'-hydroxyphenyl)benzothiazoles. The striking new features for the ESIPT photochem. and photophysics for the 4'-diethylamino derivative of 2-(2'-hydroxyphenyl)benzothiazole are discussed and MO calcs. are used to aid in the interpretation of some of the exptl. results.

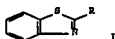
IT 10205-57-9, 2-(4'-Diethylaminophenyl)benzothiazole  
55489-32-2, 2-(2'-Hydroxy-4'-diethylaminophenyl)benzothiazole  
RL: USSES (Uses)  
(photochem. and photophysics of)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



RN 55489-32-2 HCAPLUS  
CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)

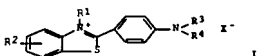


L21 ANSWER 23 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1990:440539 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 113:40539  
TITLE: An improved method for the preparation of 2-aryl-, 2-heteroaryl- and 2-styrylbenzothiazoles  
AUTHOR(S): Deligeorgiev, T. C.  
CORPORATE SOURCE: Fac. Chem., Univ. Sofia, Sofia, 1126, Bulg.  
SOURCE: Dyes and Pigments (1990), 12(4), 243-8  
CODEN: DYPIDX; ISSN: 0143-7208  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 113:40539  
OI



L21 ANSWER 24 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1989:239211 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 110:239211  
TITLE: Aqueous acid bath for the electrodeposition of brightening and leveling copper coatings  
INVENTOR(S): Dahms, Wolfgang; Seidenspinner, Hubert Matthias  
PATENT ASSIGNER(S): Schering A.-G., Fed. Rep. Ger.  
SOURCE: Eur. Pat. Appl., 10 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 297306	A1	19890104	EP 1988-108876	19880603
EP 297306	B1	19930120		
R: BR, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE				
DE 3721985	A1	19890112	DE 1987-3721985	19870630
ES 2045013	T3	19940116	ES 1988-108876	19880603
AT 8801664	A	19930515	AT 1988-1664	19880627
AT 396946	B	19931227		
JP 01100292	A	19890418	JP 1988-161089	19880630
PRIORITY APPLN. INFO.:			DE 1987-3721985	A 19870630
OTHER SOURCE(S):			CASREACT 110:239211; MARPAT 110:239211	
OI				



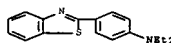
AB The bath contains at least a benzothiazolium compound (I), in which R1 = (aryl- or aralkyl-substituted) C1-5 alkyl, R2 = H, C1-5 alkyl (or alkoxy); R3 and R4 = C1-5 alkyl, and X = acid. The bath may include other additives such as poly(vinyl alc.) and thioglycolic acid. Cu is deposited at 15-45° with c.d. 0.5-12 Å/dm2.  
IT 121039-91-6  
RL: PRP (Properties)  
(electrodeposition of bright and level copper coatings from baths containing)  
RN 121039-91-6 HCAPLUS  
CN Benzothiazolium, 2-[4-(diethylamino)phenyl]-3-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

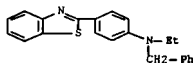
CRN 21228-90-0  
CMP C H3 O4 S

Me-O-SO3-

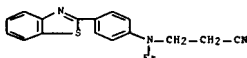
AB Cyclocondensation reaction of 24 RCHO (R = aryl, heteroaryl, cinnamyl) with 2-HSC6H4NH2 in DMSO with simultaneous removal of the volatile reaction products gives title benzothiazoles I. The procedure is simple and gives higher yields in shorter times than other procedures.  
IT 10205-57-9P 55489-36-6P 127868-58-OP  
127868-59-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



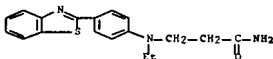
RN 55489-36-6 HCAPLUS  
CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-ethyl- (9CI) (CA INDEX NAME)



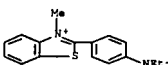
RN 127868-58-0 HCAPLUS  
CN Propanenitrile, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)



RN 127868-59-1 HCAPLUS  
CN Propanamide, 3-[[4-(2-benzothiazolyl)phenyl]ethylamino]- (9CI) (CA INDEX NAME)



CM 2  
CRN 20096-16-6  
CMP C18 H21 N2 S

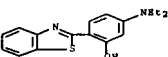


L21 ANSWER 25 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1988:482965 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 109:82965  
TITLE: Removable guidepath for automated guidance vehicles  
INVENTOR(S): Paske, Richard, Jr.; Pallmer, Michael; King, William L., Jr.  
PATENT ASSIGNER(S): Bell and Howell Co., USA  
SOURCE: U.S., 10 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4707297	A	19871117	US 1986-057729	19860429
PRIORITY APPLN. INFO.:			US 1986-057729	19860429

AB Guidepath compns., capable of producing emitted radiation detectable by automated guidance vehicles, comprise an aqueous dispersion of a fluorescent or phosphorescent compound and 55 weight% of a binder including a reversibly crosslinked ionomer. Guidepath compns. prepared using 2-(2-(naphthylsulfonylamino)phenyl-4H-3,1-benzoxazin-4-one as the fluorescent compound and Rhoplex B-1604 ionomer emulsion were applied to a variety of carpets and showed fair visual aesthetics, good durability (over 3 mo), and excellent deactivation characteristics (using a proprietary deactivation formula) on most carpets tested.

IT 55489-32-2  
RL: PRP (Properties)  
(guidepath compns. containing reversibly crosslinked ionomers and, for automated guidance vehicles)  
RN 55489-32-2 HCAPLUS  
CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)

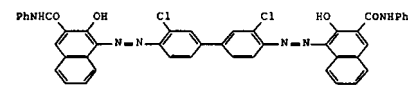


L21 ANSWER 26 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1987:93611 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 106:93611  
TITLE: Laminated sensitive materials in electrophotography

INVENTOR(S): Ishikawa, Shozo; Fujimura, Naoto  
 PATENT ASSIGNER(S): Canon K. K., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61129650	A	19860617	JP 1984-250619	19841129
PRIORITY APPLN. INFO.:			JP 1984-250619	19841129

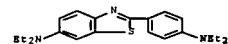
GI



11

AB Laminated sensitive materials in electrophotography contain pos.-hole-transferable charge-transport layers with charge-transport materials of the formula R(CH<sub>2</sub>CH)<sub>n</sub>NR<sub>1</sub> (I; R = heterocyclyl, anthryl; R<sub>1</sub> = aryl; n = 0-2). The materials show good sensitivity and durability. Thus, a laminated sensitive material prepared by using the charge-transport material I (R = 9-anthryl; R<sub>1</sub> = p-C<sub>6</sub>H<sub>4</sub>NEt<sub>2</sub>; n = 1) and the azo dye II was applied to an electrostatic copying process to show a good pos.-charging property and good sensitivity and durability.

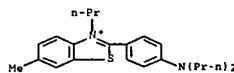
IT 74839-88-6  
 RL: USES (Uses)  
 (electrophotog. photoconductor with charge-transport material from)  
 RN 74839-88-6 HCAPLUS  
 CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 27 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1986:474404 HCAPLUS Full-text  
 DOCUMENT NUMBER: 105:74404  
 TITLE: Phenylbenzothiazolium salts as nonselective herbicides  
 INVENTOR(S): Kitaguchi, Nobuya; Shimizu, Toshio  
 PATENT ASSIGNER(S): Asahi Chemical Industry Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60084304	A	19850513	JP 1983-192212	19831014
JP 06029285	B	19940420		
AU 8434015	A	19850418	AU 1984-34015	19841008
AU 563655	B2	19870716		
CA 1230004	A1	19871208	CA 1984-465081	19841010
US 4594310	A	19860610	US 1984-660088	19841012
PRIORITY APPLN. INFO.:			JP 1983-192212	A 19831014

JP 61072703 A 19860414 JP 1984-194852 19840919  
 PRIORITY APPLN. INFO.: JP 1984-194852 19840919  
 AB 2-Phenylbenzothiazolium salts are nonselective herbicides. Thus, 2-(4'-dimethylaminophenyl)-3,6-dimethylbenzothiazolium chloride (25 g/are) was phytotoxic to Brassica rapa perrivida and controlled broad-leaf weeds.  
 IT 103678-86-0  
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)  
 (herbicide)  
 RN 103678-86-0 HCAPLUS  
 CN Benzothiazolium, 2-[4-(dipropylamino)phenyl]-6-methyl-3-propyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>+</sup>

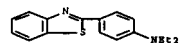
L21 ANSWER 28 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1985:532393 HCAPLUS Full-text  
 DOCUMENT NUMBER: 103:132393  
 TITLE: Photopolymerizable composition  
 INVENTOR(S): Nagasaka, Hideki  
 PATENT ASSIGNER(S): Mitsubishi Chemical Industries Co., Ltd., Japan  
 SOURCE: Bur. Pat. Appl., 22 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 138187	A2	19850424	EP 1984-112103	19841009
EP 138187	A3	19850828		
EP 138187	B1	19890111		
R: DE, FR, GB, NL				
JP 60084304	A	19850513	JP 1983-192212	19831014
JP 06029285	B	19940420		
AU 8434015	A	19850418	AU 1984-34015	19841008
AU 563655	B2	19870716		
CA 1230004	A1	19871208	CA 1984-465081	19841010
US 4594310	A	19860610	US 1984-660088	19841012
PRIORITY APPLN. INFO.:			JP 1983-192212	A 19831014

OTHER SOURCE(S): MARPAT 103:132393  
 GI For diagram(s), see printed CA issue.  
 AB A photosensitive composition is described which is highly sensitive to UV and useful for imaging applications (lithog. printing plate fabrication, relief printing plate fabrication, photoresists for printed circuits, photocurable ink, paint, adhesive, etc.). The composition contains 21 ethylenically unsatd. double bond, and a photoinitiator comprising a compound of the formula I (R,R<sub>1</sub> = alkyl; A = aromatic ring containing N; n = 1,2,3) and hexaarylbiimidazole. The initiator may addnl. contain a thiol II (Z = O,S,NH).

Thus, an anodized Al support was coated with a solution containing a copolymer of Me methacrylate and methacrylic acid (obtained by hydrolyzing PMAA), 5, trimethylolpropane triacrylate 5 g, Victoria pure blue 30, p-methoxyphenol 30 mg, MeCOEt 90 g, II 2.5, 2,2'-bis-(o-chlorophenyl)-4,4',5,5'-tetrabimidazole 5, 2-mercaptobenzothiazole 34, dried at 80° for 5 min to obtain a dry film of 2 μm, overcoated with poly(vinyl alc.) overcoat, dried, imagewise exposed, developed with an aqueous solution of 9 weight% Bu cellosolve and 1 weight% Na silicate. A relative sensitivity of the plate (measured after exposure with a high pressure Hg lamp which irradiates multilines of 366, 405 and 436 nm) was 8.0 compared to 1.0 for a composition using Michler's ketone and benzophenone as initiators.

IT 10205-57-9  
 RL: USES (Uses)  
 (photopolymerizable imaging composition initiator system containing hexaarylbiimidazole and)  
 RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



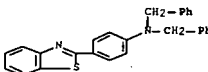
L21 ANSWER 29 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1985:158128 HCAPLUS Full-text  
 DOCUMENT NUMBER: 102:158128  
 TITLE: Two component diazo material  
 INVENTOR(S): Scheler, Siegfried  
 PATENT ASSIGNER(S): Hoechst A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 47 pp.  
 CODEN: GWXJEX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3307364	A1	19840906	DE 1983-3307364	19831002
ES 529801	A1	19850316	ES 1984-529801	19840216
EP 118086	A2	19840912	EP 1984-101944	19840224
EP 118086	A3	19870527		
EP 118086	B1	19890927		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 46773	T	19891015	AT 1984-101944	19840224
DK 8401054	A	19840903	DK 1984-1054	19840227
NO 8400758	A	19840903	NO 1984-758	19840228
JP 59165050	A	19840918	JP 1984-35467	19840228
US 4540648	A	19850910	US 1984-584547	19840228
CA 1211977	A1	19860930	CA 1984-448420	19840228
FI 8400810	A	19840903	FI 1984-810	19840229
FI 74825	B	19871130		
FI 74825	C	19880310		
ZA 8401513	A	19841031	ZA 1984-1513	19840229
BR 8400996	A	19841009	BR 1984-996	19840301
PRIORITY APPLN. INFO.:			DE 1983-3307364	A 19830302
OTHER SOURCE(S):			EP 1984-101944	A 19840224

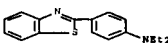
GI

AB A 2-component diazo copying material having a flat gradation and that can be used for the reproduction of halftone originals without any appreciable loss in copying speed contains a support coated with a photosensitive layer containing a diazonium salt, a coupler, an acid stabilizer, and a salt of a benzothiazole derivative (I; R = H, alkyl, or aryl; R<sub>1</sub> = H, or optionally substituted alkyl, aralkyl, aryl, pyridylalkyl, carboxyl, carboxyalkyl, carboxyaryl, carbamoyl, or sulfamoyl, or R<sub>1</sub> and R together form a heterocyclic ring; R<sub>2</sub> = H or alkyl) that absorbs in the UV region and upon treatment with an alkaline medium is converted to a nonabsorbing leuco base form. Thus, a glass-clear PET support was coated with a composition containing cellulose acetate propionate 14.00, Me<sub>2</sub>CO 135.00, MeOH 35.00, Me glycol 8.00, BuOH 8.00, S-sulfosalicylic acid 0.41, 2-hydroxy-3-naphthoic acid N-(2-methoxyphenyl) amide 0.88, 1-hydroxy-2-naphthoic acid N-piperidine 0.60, 2,5-diethoxy-4-N-morpholinobenzene diazonium tetrafluoroborate 1.56 g, and 6-methyl-2-(4-aminophenyl)benzothiazole 10 weight% (based on the above diazonium salt), dried 1 min at 100°, exposed, and processed to show an effect copying speed of 71% and a clear flattening of the gradation.

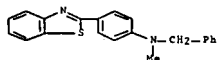
IT 55489-35-5  
 RL: USES (Uses)  
 (diazo copying materials containing, as UV light-absorbing agent for images with flat gradation)  
 RN 55489-35-5 HCAPLUS  
 CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



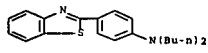
IT 10205-57-9P 55489-34-4P 95856-74-9P  
 95856-77-2P 95856-81-0P  
 RL: PREP (Preparation)  
 (preparation and UV light absorber applications of, in diazo copying materials)  
 RN 10205-57-9 HCAPLUS  
 CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 55489-34-4 HCAPLUS  
 CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-methyl- (9CI) (CA INDEX NAME)

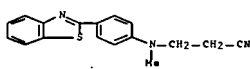


RN 95856-74-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-dibutyl-, monohydrochloride (9CI) (CA INDEX NAME)

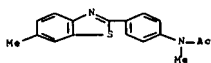


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RN 95856-77-2 HCAPLUS  
CN Propanenitrile, 3-[(4-(2-benzothiazolyl)phenyl)methylamino]- (9CI) (CA INDEX NAME)



RN 95856-81-8 HCAPLUS  
CN Acetamide, N-methyl-N-[4-(6-methyl-2-benzothiazolyl)phenyl]- (9CI) (CA INDEX NAME)



L21 ANSWER 30 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1985:112727 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 102:112727  
TITLE: Solid-state fluorescent photophysics of some 2-substituted benzothiazoles  
AUTHOR(S): Anthony, Kevin; Brown, Robert G.; Hepworth, John D.; Hodgson, Kevin W.; May, Bernadette; West, Michael A.  
CORPORATE SOURCE: Sch. Chem., Lancashire Polytech., Preston, PR1 2TQ, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1984), (12), 2111-17  
CODEN: JCPKHH; ISSN: 0300-9580

TITLE: Halochromic molecules. Part 4. Chromogenic compounds by cyclization of [2-(2-benzothiazolylamino)-4-(diethylamino)phenyl]heteroarylium salts: synthesis and acidobasic behavior  
AUTHOR(S): Ziegler, Hugo; Balli, Heinz  
CORPORATE SOURCE: Inst. Farbenchem., Univ. Basel, Basel, CH-4056, Switz.  
SOURCE: Helvetica Chimica Acta (1983), 66(7), 2165-81  
CODEN: HCACAV; ISSN: 0018-019X  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 100:87232  
GI For diagram(s), see printed CA issue.  
AB Colored [2-(2-benzothiazolylamino)-4-(diethylamino)phenyl]heteroarylium salts (I; A = 2,6-diphenylpyrylium-4-yl, 2,6-diphenylthiopyrylium, 3-ethylbenzothiazolium-2-yl, 1-ethylquinolinium-2 (and 4-yl) are deprotonated to colorless spiro compds. (II; A = 2,6-diphenylpyran-4-ylidene, etc.). The synthesis of I and II from 2-[3-(diethylamino)anilino]benzothiazole [88760-92-3] is described, and their structures were elucidated by 1H-NMR and UV-visible spectroscopy. The halochromic properties were studied by spectrophotometric determination of  $\epsilon_{\text{ph}}$  and  $\epsilon_{\text{ho}}$  curves in buffered MeOH-H<sub>2</sub>O solution.  $\text{pK}^{\text{a}}$  values were also determined and the complex protonation equilibrium discussed. A tautomer of I (A = 5-phenyl-1,2-dithiolium-3-yl) did not form the corresponding II when deprotonated but instead was stabilized by  $\sigma$ -bond resonance.  
IT 88851-47-2 89960-01-9  
RL: PRP (Properties)  
(NMR spectrum of)  
RN 88851-47-2 HCAPLUS  
CN Benzothiazolium, 2-[4-(diethylamino)-2-[(3-ethyl-2(3H)-benzothiazolylidene)amino]phenyl]-3-ethyl-, tetrafluoroborate(1-), mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 76-05-1  
CMP C2 H F3 O2



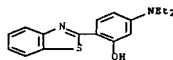
CM 2

CRN 88851-39-2  
CMP C28 H31 N4 S2 . B F4

CM 3

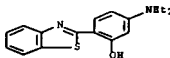
CRN 88851-38-1  
CMP C28 H31 N4 S2

DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The solid-state fluorescence was examined of 39 benzothiazoles with a Ph, naphthyl or coumarin substituent in the 2-position. The necessity of a 2'-OH substituent for fluorescence was confirmed, and the effects of further substitution in the 2-Ph ring are reported.  
IT 55489-32-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and fluorescence of)  
RN 55489-32-2 HCAPLUS  
CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)

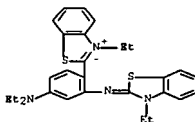


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L21 ANSWER 31 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1984:454389 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 101:54389  
TITLE: Determination of the fluorescence quantum yields of some 2-substituted benzothiazoles  
AUTHOR(S): Kirkbright, G. F.; Spillane, D. E. M.; Anthony, Kevin; Brown, R. G.; Hepworth, J. D.; Hodgson, K. W.; West, M. A.  
CORPORATE SOURCE: Inst. Sci. Technol., Univ. Manchester, Manchester, M60 1QD, UK  
SOURCE: Analytical Chemistry (1984), 56(9), 1644-7  
CODEN: ANCHAM; ISSN: 0003-2700  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Fluorescence quantum yields were determined for numerous solid title compds. by a conventional optical method and by photoacoustic spectroscopy. The quantum yields measured by the latter method were consistently higher, although in most cases there was agreement to within 0.1. The principal cause of the variation was measurement error in one or both systems.  
IT 55489-32-2  
RL: PRP (Properties)  
(fluorescence of, optical and photoacoustic determination of)  
RN 55489-32-2 HCAPLUS  
CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



L21 ANSWER 32 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1984:87232 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 100:87232



CM 4

CRN 14874-70-5  
CMP B F4  
CCI CCS



RN 88860-01-9 HCAPLUS  
CN Benzothiazolium, 2-[2-(2-benzothiazolylamino)-4-(diethylamino)phenyl]-3-ethyl-, tetrafluoroborate(1-), mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 76-05-1  
CMP C2 H F3 O2

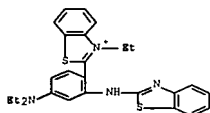


CM 2

CRN 88851-24-5  
CMP C26 H27 N4 S2 . B F4

CM 3

CRN 88851-23-4  
CMP C26 H27 N4 S2



CM 4

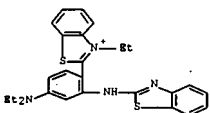
CRN 14874-70-5  
 CMP B F4  
 CCI CCS



IT 88851-24-5P 88851-39-2P  
 RL: PRP (Properties); SPN (Synthetic preparation); PRSP (Preparation)  
 (preparation and NMR spectrum of)  
 RN 88851-24-5 HCAPLUS  
 CN Benzothiazolium, 2-[(2-(2-benzothiazolylamino)-4-(diethylamino)phenyl)-3-ethyl-, tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 88851-23-4  
 CMP C26 H27 N4 S2



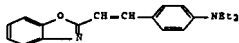
CM 2

CRN 14874-70-5  
 CMP B F4  
 CCI CCS

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 92255	A1	19831026	EP 1983-103889	19830420
EP 92255	B1	19870114		
R: DE, FR, GB, IT				
JP 56182640	A	19831025	JP 1982-66964	19820420
JP 0306382	B	19910410	US 1985-695575	19850128
US 4619879	A	19861028	JP 1982-66964	A 19820420
PRIORITY APPLN. INFO.:				
			US 1983-486821	A1 19830420

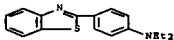
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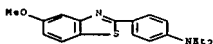
AB An electrophotog. photoconductor which exhibits high sensitivity to light emitted by the semiconductor lasers comprises a charge-generating layer containing metal-free phthalocyanine and a charge-transport layer containing a nonionic compound of styrylic or oxazole dye base. Thus, an Al foil support was coated with a mixture containing t-form metal-free phthalocyanine 1 and a butyral resin (XYHL) (6% solution in xylene) 1 part to form a dry 3 μ layer and overcoated with a mixture containing 1 1.5, a polycarbonate resin 1, CH2Cl2 10.10, and 1,2-dichloroethane 3 parts to give a 13 μ thick charge-transport layer. The obtained photoreceptor was subjected to 10 s corona discharge at -5 kV and exposed to a W lamp. The initial surface potential of the photoreceptor was 850 V, the white light sensitivity was 0.8 lx·s, and the dark decay was 74%. Its spectral sensitivity extended from 550 to 800 nm.

IT 10205-57-9 76869-48-2  
 RL: USES (Uses)  
 (electrophotog. photoreceptor with charge generating layer containing metal-free phthalocyanine and charge transport layer containing, spectral sensitivity of, in visible and IR region)

RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



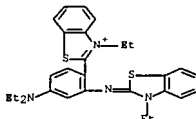
RN 76869-48-2 HCAPLUS  
 CN Benzenamine, N,N-diethyl-4-(5-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 88851-39-2 HCAPLUS  
 CN Benzothiazolium, 2-[(4-(diethylamino)-2-[(3-ethyl-2(3H)-benzothiazolylidene)amino]phenyl)-3-ethyl-, tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 88851-38-1  
 CMP C28 H31 N4 S2



CM 2

CRN 14874-70-5  
 CMP B F4  
 CCI CCS

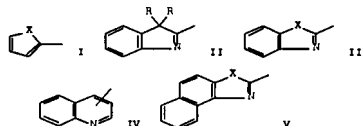


L21 ANSWER 33 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1984:43058 HCAPLUS Full-text  
 DOCUMENT NUMBER: 100:43058  
 TITLE: Composite type photosensitive member for electrophotography  
 INVENTOR(S): Kakuta, Atsushi; Oka, Hiroyuki; Suzuki, Shigeo; Araya, Kotaro; Mori, Yasuki; Morishita, Hirosada  
 PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 42 pp.  
 CODEN: SPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1

L21 ANSWER 34 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1982:627496 HCAPLUS Full-text  
 DOCUMENT NUMBER: 97:227496  
 TITLE: Complex type electrophotographic plates  
 INVENTOR(S): Kakuta, Atsushi; Suzuki, Shigeo; Mori, Yasuki; Morishita, Hirosada  
 PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
 SOURCE: U.S., 20 pp. Cont.-in-part of U.S. Ser. No. 70,822, abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2

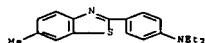
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4346157	A	19820824	US 1981-232829	19810209
JP 55035319	A	19800312	JP 1978-107466	19780904
JP 60008500	B	19850304		
JP 55064243	A	19800514	JP 1978-136697	19781108
PRIORITY APPLN. INFO.:				
			JP 1978-107466	A 19780904
			JP 1978-136697	A 19781108
			US 1979-70822	A2 19790829

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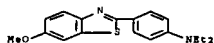


AB Complex-type electrophotog. plates are described which consist of a conductive support, a 1st layer of a charge-generating material with a thickness of 0.1 to 5 μm and a 2nd layer of a homogeneous mixture of a charge-transport material with the general formula R(CH:CH)nR1 (R = I, II, III, IV, or V where X = 0 or S; R1 = aryl or substituted aryl; R2 = alkyl; n = 0, 1, or 2) and an insulating, resinous binder with a thickness of 5 to 100 μm. The resultant plates have a high light sensitivity and can be used in >103 cycles without fatigue. Thus, a 1% solution of Chlorodian Blue in ethylenediamine was coated on an Al-coated polyester film to give a charge-generating layer with a 1μ thickness. Then a 1% dichloromethane solution of a 2-(p-diethylaminostyryl)benzoxazole-lupilon 52000 (polycarbonate resin) (1:2) mixture was coated thereon to give a charge transport layer with a 30μ thickness. The resulting electrophotog. plate showed satisfactory characteristics and durability.

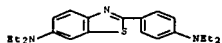
IT 10205-63-7 10205-72-6 74839-89-6  
 RL: USES (Uses)  
 (electrophotog. plate with charge-transport layer containing)  
 RN 10205-63-7 HCAPLUS  
 CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 10205-72-8 HCAPLUS  
CN Benzenamine, N,N-diethyl-4-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 74839-88-6 HCAPLUS  
CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-diethyl- (9CI) (CA INDEX NAME)

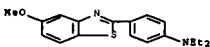


L21 ANSWER 35 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1982:78635 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 96:78635  
TITLE: Photoelectric cell  
PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56133879	A	19811020	JP 1980-36055	19800324
			JP 1980-36055	A 19800324

PRIORITY APPLN. INFO.:  
AB In a photoelec. cell with a 1st electrode contacting an impurity region in a semiconductor substrate, a photoelec.-conversion region on the 1st electrode, and a transparent electrode on the photoelec.-conversion region, the photoelec. conversion region consists of a photoconductor layer from an inorg. material and semiconductor layer from an organic material. The cell is useful in pickup tubes.  
IT 10205-57-9  
RL: USES (Uses)  
(semiconductor layers from, for photoelec. cells)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

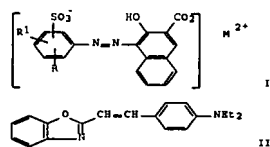
RN 76869-48-2 HCAPLUS  
CN Benzenamine, N,N-diethyl-4-(5-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



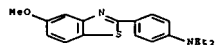
L21 ANSWER 37 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1981:45268 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 95:52658  
TITLE: Composite electrophotographic plates  
PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56005548	A	19810121	JP 1979-80167	19790627
JP 60039941	B	19850713		

PRIORITY APPLN. INFO.:  
GI



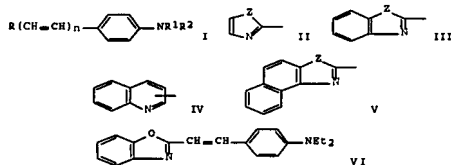
RN 76869-48-2 HCAPLUS  
CN Benzenamine, N,N-diethyl-4-(5-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



L21 ANSWER 39 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1981:217581 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 94:217581  
TITLE: Composite electrophotographic plates  
PATENT ASSIGNER(S): Hitachi, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
CODEN: JKXXAP  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

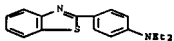
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55155358	A	19801203	JP 1979-62663	19790523
JP 62055652	B	19871120		

PRIORITY APPLN. INFO.: JP 1979-62663 A 19790523  
GI



AB A composite electrophotog. plate has a charge-generating layer containing As2Se3 and a charge-transfer layer containing a compound of the formula I (R = II, III, IV, V; R1, R2 = Me, Et, Pr; n = 0, 1, 2; Z = O, S; R may contain substituents). Thus, As2Se3 was vacuum deposited on an Al plate and overcoated with a composition containing VI and a polycarbonate resin (Supiron 2000) to give an electrophotog. plate having high sensitivity, good electrostatic characteristics and durability.  
IT 10205-57-9 76869-48-2  
RL: TEM (Technical or engineered material use); USES (Uses)

AB Composite electrophotog. plates containing Sb2S3 as the charge-generating pigment are claimed. Preferably, the electrophotog. plates contain a charge-transfer agent of the general formula R(CH=CH)nC6H4NR1R2-p (R = I, II, III, IV; Z = O, S; n = 0, 1, 2; R1, R2 = Me, Et, Pr; and the R group may contain substituents). Thus, Sb2S3 was vacuum-deposited on an Al support, and the Sb2S3 layer was overcoated with a composition containing NK 1347 (V; from Nippon Kanko Shikiso Kenkyu-sho) <S and a polycarbonate resin to give a composite electrophotog. plate having good sensitivity and durability.  
IT 10205-57-9  
RL: TEM (Technical or engineered material use); USES (Uses)  
(electrophotog. charge-transfer agent)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

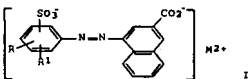


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L21 ANSWER 41 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1981:112493 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 94:112493  
TITLE: Composite electrophotographic plates  
PATENT ASSIGNER(S): Hitachi, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
CODEN: JKXXAP  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

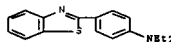
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55105251	A	19800812	JP 1979-11886	19790206
			JP 1979-11886	A 19790206

PRIORITY APPLN. INFO.:  
GI

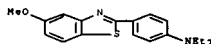


AB Composite electrophotog. plates contain charge-generating pigments of the formula I (R = H, Me, MeO, halo; R1 = Me, MeO, M2+ = divalent metal ion) and charge-transfer agents of the formula R2(CH=CH)nC6H4NR32 (II; R2 = quinolyl, oxazol-2-yl, thiazol-2-yl, benzoxazol-2-yl, benzothiazol-2-yl, naphth[1,2-d]oxazol-2-yl, naphth[1,2-d]thiazol-2-yl;

(electrophotog. charge-transfer agent)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



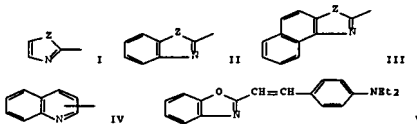
RN 76869-48-2 HCAPLUS  
CN Benzenamine, N,N-diethyl-4-(5-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



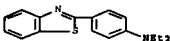
L21 ANSWER 40 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1981:130310 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 94:130310  
TITLE: Composite electrophotographic plates  
PATENT ASSIGNER(S): Hitachi, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
CODEN: JKXXAP  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55124151	A	19800925	JP 1979-29963	19790316
JP 63035023	B	19880713		

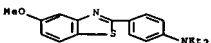
PRIORITY APPLN. INFO.: JP 1979-29963 A 19790316  
GI



R3 = Me, Et, Pr; n = 0, 1, 2). Thus, an Al plate was coated with Brilliant Carmine 6B Super (C.I. 15850), and coated with a mixture of II (R2 = benzoxazol-2-yl; R3 = Et) and a polycarbonate resin to give a high-sensitivity electrophotog. plate having good durability.  
IT 10205-57-9 76869-48-2  
RL: TEM (Technical or engineered material use); USES (Uses)  
(electrophotog charge-transfer agent)  
RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



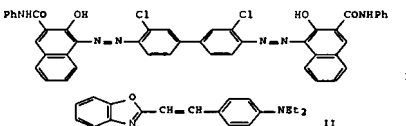
RN 76869-48-2 HCAPLUS  
CN Benzenamine, N,N-diethyl-4-(5-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



L21 ANSWER 42 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 1980:577240 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 93:177240  
TITLE: Composite type electrophotographic plates  
PATENT ASSIGNER(S): Hitachi, Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
CODEN: JKXXAP  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55053333	A	19800418	JP 1978-126202	19781016
			JP 1978-126202	A 19781016

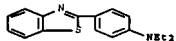
PRIORITY APPLN. INFO.:  
GI





AB In preparing an electrophotog. plate having a charge-generating agent and a charge-transfer agent, the charge-generating agent and charge-transfer agent are selected so that their colors are complementary to each other. The use of complementary color combinations results in a narrow sensitivity wavelength, and hence the electrophotog. plate becomes very useful for laser printers, etc. Thus, chlorinated Diane Blue (I; absorption maximum .smeg.600 nm) and NK-1347 (II; absorption maximum .smeg.400 nm) were used to prepare an electrophotog. plate which exhibited maximum sensitivity at .apprx.600 nm.

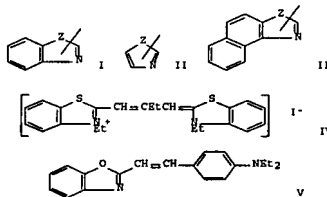
IT 10205-57-9  
 RL: USES (Uses)  
 (electrophotog. charge generating pigment-charge transfer agent combinations containing)  
 RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 43 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1980:577239 HCAPLUS Full-text  
 DOCUMENT NUMBER: 93:177239  
 TITLE: Composite electrophotographic plates  
 PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

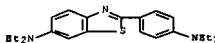
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55053334	A	19800418	JP 1978-126197	19781016
PRIORITY APPLN. INFO.:			JP 1978-126197	A 19781016

GI



AB Composite-type electrophotog. plates contain a cyanine dye as a charge-generating agent and a compound of the formula R(CH:CH)nPh [R = heterocyclic moiety selected from I, II, and III (Z = O, S, CH2, CH=CH); n = 0, 1, 2] as a charge-transfer agent. The electrophotog. plates exhibit excellent sensitivity and durability. Thus, NK 737 (IV) and V were used to prepare an electrophotog. plate having high sensitivity and durability.

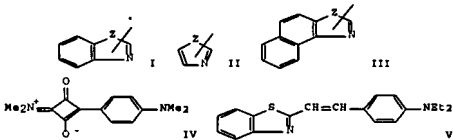
IT 74839-88-6  
 RL: USES (Uses)  
 (electrophotog. charge transfer agent)  
 RN 74839-88-6 HCAPLUS  
 CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 44 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1980:577239 HCAPLUS Full-text  
 DOCUMENT NUMBER: 93:177239  
 TITLE: Composite electrophotographic plates  
 PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

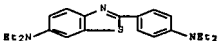
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55053335	A	19800418	JP 1978-126203	19781016
PRIORITY APPLN. INFO.:			JP 1978-126203	A 19781016

GI



AB Composite type electrophotog. materials contain squaric acid derivative methyne pigments as the charge-generating agents and comds. having general structure R(CH:CH)nPh [R = I, II, III (Z = O, S, CH2, CH=CH); n = 0, 1, 2] as the charge-transfer agents. Thus, IV and V were used to prepare an electrophotog. plate having excellent sensitivity and durability.

IT 74839-88-6  
 RL: TEM (Technical or engineered material use); USES (Uses)  
 (electrophotog. charge-transfer agent)  
 RN 74839-88-6 HCAPLUS  
 CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



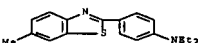
L21 ANSWER 45 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1980:540971 HCAPLUS Full-text  
 DOCUMENT NUMBER: 93:140971  
 TITLE: Electrophotographic plate  
 INVENTOR(S): Kakuta, Atsushi; Suzuki, Shigeo; Mori, Yasuki; Morishita, Hiroasada  
 PATENT ASSIGNEE(S): Hitachi, Ltd., Japan  
 SOURCE: Ger. Offen., 54 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2935481	A1	19800403	DE 1979-2935481	19790903
DE 2935481	C2	19821125		
DE 2935481	C3	19871112		
JP 55053319	A	19800312	JP 1978-107466	19780904
JP 60008500	B	19850304		
JP 55064243	A	19800514	JP 1978-136697	19781108
NL 7906570	A	19800306	NL 1979-6570	19790831
NL 174770	B	19840301		
NL 174770	C	19840801		
FR 2435073	A1	19800328	FR 1979-22031	19790903
FR 2435073	B1	19800826		

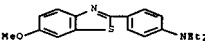
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2032637	A	19800508	GB 1979-30453	19790903
GB 2032637	B	19830112		
CH 643374	A5	19840530	CH 1979-7941	19790903
PRIORITY APPLN. INFO.:			JP 1978-107466	A 19780904
			JP 1978-136697	A 19781108

AB Electrophotog. plates of the complex type are described which consists of an elec. conductive support and a layer containing a charge-injecting material and a charge-transporting material of the general formula R(CH:CH)nR1 [R = a heterocyclic group containing N and O, S, or Se; R1 = an aryl group; n = 0-2]. These charge-transporting comds. have a m.p. of 5180°, good compatibility with polymeric comds., and good photosensitivity, resistance to fatigue, and good surface smoothness in thin films. Thus, a Metalumy film was coated with a 1% solution of chlorodiane blue in ethylenediamine to give a 1µm thick film (dry). This film was then overcoated with a 1% dichloroethane solution of a 2-(p-diethylamino)styryl)benzoxazole-Iupilon 82090 (polycarbonate resin) mixture (1:2) to give a 30µm thick film (dry). The half-value of the exposure sensitivity of the resulting electrophotog. plate was 10 lx-s. After >103 copying cycles, the plate showed no decrease in its electrophotog. characteristics.

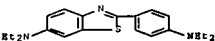
IT 10205-63-7 10205-72-8 74839-88-6  
 RL: USES (Uses)  
 (electrophotog. plate, complex, with charge-transporting layers containing)  
 RN 10205-63-7 HCAPLUS  
 CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 10205-72-8 HCAPLUS  
 CN Benzenamine, N,N-diethyl-4-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 74839-88-6 HCAPLUS  
 CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 46 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1980:102294 HCAPLUS Full-text  
 DOCUMENT NUMBER: 92:102294  
 TITLE: Electrophotographic photosensitive materials  
 INVENTOR(S): Sasaki, Masao; Ohta, Masafumi; Tetsui, Kyoji

PATENT ASSIGNER(S): Hashimoto, Mitsuru; Sakai, Kiyoshi; Kazami, Takeo  
 SOURCE: Ricoh Co., Ltd., Japan  
 Jpn. Kokai Tokkyo Koho, 30 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54061936	A	19790518	JP 1977-128448	19771026
PRIORITY APPL. INFO.			JP 1977-128448	A 19771026

GI For diagram(s), see printed CA issue.

AB Charge-carrier-transferring agents for electrophotog. photosensitive materials are selected from the following groups of compds. (1) Compds. of the general formulas I and II (R = H, alkyl, acetyl, cycloalkyl; R1 = alkyl, R2 = alkyl, acetyl; R3 = H, alkyl). (2) Compds. of the general formula IV (R4, R5 = Ph or Ph group substituted with 21 of halo, amino, C1-4 alkyl, OH, C1-4 alkoxy substituents; R6, R7 = H, C1-4 alkyl, Ph, substituted phenyl; Z = O, S). (3) Compds. of the general formula IV (R8 = H, alkyl, alkenyl, aralkyl, aralkenyl, aryl, substituted aryl, heterocyclic moiety; R9, R10 = Ph, substituted Ph). (4) Compds. of general formulas V, VI, VII, and VII (R11 = aminophenyl, alkylaminophenyl; R12 = Ph, substituted Ph; R13 = H, alkyl, alkenyl, heterocyclic moiety; R14, R15 = Ph, substituted Ph; 1 of R14 and R15 is alkylaminophenyl or aminophenyl; R16 = H, alkyl). (5) Compds. of the general formula IX [21 = group of atoms required to form aromatic ring; 22 = O, S, NR17 (R17 = H, alkyl, aryl, aralkyl); R18 = aromatic or heterocyclic moiety]. (6) Compds. of the general formula R19CONHN:CR2OR21 (R19 = H, alkyl, aralkyl, aryl, substituted aryl, aromatic heterocyclic moiety; R20 = aralkyl, aryl, substituted aryl, aromatic heterocyclic moiety; R21 = H, alkyl, aryl, substituted aryl; R2OR21 in combination may complete a C ring together with the C atom). (7) Compds. of the general formula R22CH:CR23R24 (R22 = aromatic C ring, aromatic heterocyclic moiety, styryl; R23 = H, acyl, amino; R24 = aromatic C ring moiety, aromatic heterocyclic moiety, carbalkoxy, carbamido, CN). (8) Compds. of the formula X (R25, R26 = aromatic or heterocyclic moiety, R27 = H, aliphatic moiety; R28 = H, aromatic moiety, heterocyclic moiety). (9) Compds. of the formula XI (R29, R30 = H, C1-6 alkyl, branched alkyl (56 C atoms in the longest chain)). (10) The compound XII. And (11) compds. of the general formula XIII (R31 = Me, Et, Pr, MeO; R32 = Cl, MeO; m = 0, 1; n = 0, 1, 2) or XIV (R33 = Me, Et, MeO; R34 = Cl, MeO; m = 0, 1; n = 0, 1, 2). Thus, an electrophotog. plate prepared by using Diane Blue (as the charge-carrier-generating pigment) and 2,5-bis(4-(ethylamino)phenyl)-1,3,4-triazole (as the charge-carrier-transfer agent) had a E1/2 sensitivity of 4.1 lx.s.

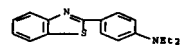
IT 10205-57-9

RL: USES (Uses)

(electrophotog. charge carrier transfer agent)

RN 10205-57-9 HCAPLUS

CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 47 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1979:438673 HCAPLUS Full-text

DOCUMENT NUMBER: 91:38673

TITLE: IR-spectra and calculation of the  $\pi$ -electron

structure of some thiazolylazo compounds

AUTHOR(S): Olenovich, N. L.; Tantsyura, G. P.; Lozitskaya, E. P.;

Savenko, G. I.; Malakhova, N. M.

GI For diagram(s), see printed CA issue.

AB The colorless benzoxazoles I (R = H, OH, or Me; R1 = H, Me, Et, or CH2Ph; R2 = e.g. H, Me, Et, CH2Ph, or Ph; R3 = H, Me, OMe, NMe2, or Cl; X = O or S), giving yellow shades on copying paper on contacting with acids, were prepared. Thus, refluxing 2-H2NC6H4SH [137-07-5] with 4-PhMeNC6H4CHO [55489-38-8] 4 hr in HOAc gave colorless color former (I, R = R3 = H, R1 = Me, R2 = Ph, X = S) [55489-39-9]. Similarly prepared were 23 other I.

IT 10205-57-9P 10205-63-7P 10205-72-8P

10205-78-4P 55489-32-2P 55489-34-4P

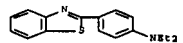
55489-35-5P 55489-36-6P

RL: IMP (Industrial manufacture); PREP (Preparation)

(preparation of, color formers, for copying paper)

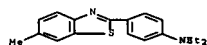
RN 10205-57-9 HCAPLUS

CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



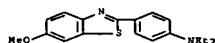
RN 10205-63-7 HCAPLUS

CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



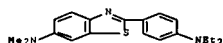
RN 10205-72-8 HCAPLUS

CN Benzenamine, N,N-diethyl-4-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 10205-78-4 HCAPLUS

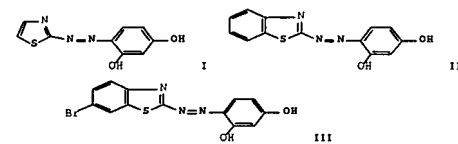
CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 55489-32-2 HCAPLUS

CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)

CORPORATE SOURCE: Odessa Univ., Odessa, USSR  
 SOURCE: Voprosy Stereokhimii (1978), 7, 62-7  
 CODEN: VSTKB9; ISSN: 0372-6762  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI



AB I, II, III and the corresponding 1-substituted 2-naphthols and 6-substituted 3-Rt2NC6H4OH analogs existed in 2 tautomeric forms, as shown by IR and MO calcs. With metals the compds. acted as tridentate ligands and formed 2 rings.

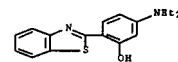
IT 55489-32-2

RL: PRP (Properties)

(tautomerization and complexing properties of, IR and MO calcs. in relation to)

RN 55489-32-2 HCAPLUS

CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



L21 ANSWER 48 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1975:429894 HCAPLUS Full-text

DOCUMENT NUMBER: 83:29894

TITLE: Benzoxazoles and benzothiazoles for copying paper

INVENTOR(S): Oberlinner, Andreas

PATENT ASSIGNER(S): BASF A.-G.

SOURCE: Ger. Offen., 10 pp.

CODEN: GWXIBX

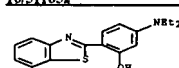
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

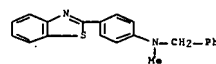
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2333378	A1	19750123	DE 1973-2333378	19730630
PRIORITY APPL. INFO.			DE 1973-2333378	A 19730630



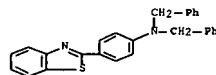
RN 55489-34-4 HCAPLUS

CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-methyl- (9CI) (CA INDEX NAME)



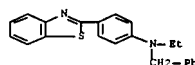
RN 55489-35-5 HCAPLUS

CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 55489-36-6 HCAPLUS

CN Benzenemethanamine, N-[4-(2-benzothiazolyl)phenyl]-N-ethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 49 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1974:484424 HCAPLUS Full-text

DOCUMENT NUMBER: 81:04424

TITLE: Storage and retrieval of information

PATENT ASSIGNER(S): Kalle A.-G.

SOURCE: Fr. Denende, 12 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

10/511852 173/217 Robert Havlin

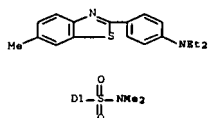
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2173237	A1	19731005	FR 1973-6461	19730223
FR 2173237	B1	19770729		
DE 2208727	A1	19731004	DE 1972-2208727	19720224
DE 2208727	B2	19800814		
DE 2208727	C3	19810423		

PRIORITY APPLN. INFO.: DE 1972-2208727 A 19720224

AB Recording is made by using an electron beam to form a latent image in a photoconductive layer. The latent image is made visible by uniformly charging the surface in an elec. field and developing with a toner or by scanning with a low-power electron beam and using the elec. current produced in the photoconductive layer at each instant to drive a synchronized cathode ray tube or to record on a magnetic tape. Thus, an aluminized polyester support was coated with a composition prepared from poly(vinylcarbazole) 19.3, trinitrofluorenone 31.5, isophthalic acid-terephthalic acid copolymer 4.2 and THF 545 g to give a 15 µ layer, exposed by a 0.5 W-sec/cm<sup>2</sup> electron beam producing a latent image, charged to 800 V, imaged for 0.5 sec to a 15 W M-lamp at 20 cm, developed with a toner, and the toner image was transferred to a receptor paper.

IT 53694-00-1  
RL: USSES (Uses)  
(photoconductive comps. containing, for electron beam recording)

RN 53694-00-1 HCAPLUS  
CN Benzoethiazolesulfonamide, 2-[4-(diethylamino)phenyl]-N,N,6-trimethyl- (9CI) (CA INDEX NAME)



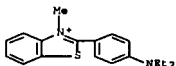
L21 ANSWER 50 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1973:499179 HCAPLUS Full-text  
DOCUMENT NUMBER: 79:99179  
TITLE: New free-radical color films  
AUTHOR(S): Sprague, Robert H.; Rorke, Phyllis  
CORPORATE SOURCE: Itek Corp., Lexington, MA, USA  
SOURCE: Unconventional Photogr. Syst., Symp., 3rd (1971), 65-7. Editor(s): Conger, Richard R. Soc. Photogr. Sci. Eng.: Washington, D. C.  
CODEN: 26XCAP  
DOCUMENT TYPE: Conference  
LANGUAGE: English

GI For diagram(s), see printed CA issue.

AB The dye precursors, I (cyan, maximum sensitivity at 445 nm), II (magenta, maximum sensitivity at 425 nm), and III (yellow, maximum sensitivity at 390 nm) complexed with the activators CB4 or tribromoacetophenone, are exposed to light. HBr from the activator reacts with the precursor to form the colored dye salt. The precursor is soluble in PhMe; the dye salt is not. The coatings are usually prepared with polystyrene as the film-forming binder and applied to polyester film supports. A poly(vinyl butyral) coating that contains phthalic acid (mordant) is a receptor for the pos. dye image. This subtractive color reproduction process is suitable for gravure, halftone work, and proofs of both pos. and neg. seps.; pos. color prints can also be prepared

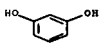
IT 50481-81-9  
RL: USSES (Uses)

10/511852 175/217 Robert Havlin



• Cl<sup>-</sup>

CM 2  
CRN 108-46-3  
CMP C6 H6 O2



L21 ANSWER 52 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1967:106008 HCAPLUS Full-text  
DOCUMENT NUMBER: 66:106008  
TITLE: Coatings for electrophotographic processes  
INVENTOR(S): Kowche, Horst  
PATENT ASSIGNEE(S): Renker-Belipe G.m.b.H.  
SOURCE: U.S., 12 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3300304		19670124	US 1961-146398	19611002
				19601003

PRIORITY APPLN. INFO.: DE

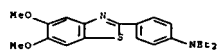
AB The coating materials for electrophotographic processes usually consist of a combination of a photoconductor and an insulating binder. It is possible to combine known photoconductors with epoxy or organic isocyanate deriva. to give photoconducting resins that require no binder. Suitable photoconductors include 1,3,4-oxadiazoles, 1,3,4-triazoles, azomethines, acylhydrazones, oxanilines, thiazoles, thio ketones, and organometallic comds. Thus, 90 g. Desmodur L (75% modified triisocyanate in EtOAc) is added to 40 g. 2-(4-aminophenyl)-6-methylbenzothiazole in 750 ml. dry cyclohexanone, boiled to remove the EtOAc, and refluxed at 155° for 30 min. The product, which sep. after standing overnight, was washed with cold Me<sub>2</sub>CO, dissolved in 250 ml. cyclohexane, mixed with 20 ml. ethylene glycol, and heated to 125° for 30 min. The resultant resin solution was thinned with 100 ml. MeCOEt, coated onto Al plates, dried, and baked at 130-40° for 30 min. to give a scratch-resistant, sparingly soluble photoconducting layer that can be exposed, developed, and fixed or transferred by conventional techniques, and also withstands washing and re-use.

IT 31668-76-5  
RL: USSES (Uses)  
(coatings of, on aluminum plates, for electrophotography)

RN 31668-76-5 HCAPLUS  
CN Phenol, 4,4'-isopropylidenedi-, polymer with 6-amino-2-[p-

10/511852 174/217 Robert Havlin

(dye precursor, in free-radical color photog. films)  
RN 50481-83-9 HCAPLUS  
CN Benzenamine, 4-(5,6-dimethoxy-2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

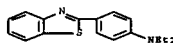


L21 ANSWER 51 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1969:47348 HCAPLUS Full-text  
DOCUMENT NUMBER: 70:47348  
TITLE: Anthelmintic quaternary salts. III. Benzoethiazolium salts  
AUTHOR(S): Garmaise, David L.; Paris, Gérard Y.; Komlosy, Jacqueline; Chambers, C. H.; McCrae, R. C.  
CORPORATE SOURCE: Res. Dep., Abbott Lab. Ltd., Montreal, Can.  
SOURCE: Journal of Medicinal Chemistry (1969), 12(1), 30-6  
CODEN: JMCMAH; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 70:47348

AB The synthesis and anthelmintic activity of a number of benzoethiazolium salts analogous to the dye thioflavin T are described. The structural requirements for activity include a 2-phenyl substituent with a basic group in the para position, and a 3-alkyl group no larger than Et (preferably Me). The isomeric salts in which the site of quaternization is the exocyclic N, as well as the unquaternized benzoethiazoles, are devoid of activity. The benzoethiazole nucleus may be substituted with alkyl, alkoxy, or methylthio groups, but not with halogen. The most active comds. are of interest because they provide both lung and liver protection to swine by inhibiting the migration of Ascaris suum larvae in swine. Thioflavin and 2 analogs also showed activity against gastrointestinal nematodes in sheep.

IT 10205-57-9P 20135-34-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 10205-57-9 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



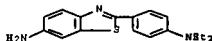
RN 20135-34-6 HCAPLUS  
CN Benzoethiazolium, 2-(4-(diethylamino)phenyl)-3-methyl-, chloride, compd. with 1,3-benzenediol (1:1) (9CI) (CA INDEX NAME)

CM 1  
CRN 20096-10-0  
CMP C18 H21 N2 S . Cl

10/511852 176/217 Robert Havlin

(diethylamino)phenylbenzothiazole and 1-chloro-2,3-epoxypropane (8CI)  
(CA INDEX NAME)

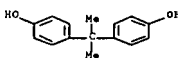
CM 1  
CRN 5809-18-7  
CMP C17 H19 N3 S



CM 2  
CRN 106-89-8  
CMP C3 H5 Cl O



CM 3  
CRN 80-05-7  
CMP C15 H16 O2



L21 ANSWER 53 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1967:7123 HCAPLUS Full-text  
DOCUMENT NUMBER: 66:7123  
TITLE: Supersensitized zinc oxide  
INVENTOR(S): Clausen, Ralph L.; Meyer, Donald K.  
PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co.  
SOURCE: U.S.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3712144		19660906	US	19611211

AB A method is described for the preparation of supersensitized ZnO and its use as a photoconductor in the preparation of improved photoconductor sheets for use in the visible region. Sensitization of ZnO is accomplished when the ZnO surface contains, in addition to a sensitizing dye, a colorless complex of Zn<sup>2+</sup> and a complexing agent such as 2-(4-dimethylaminophenyl)-3,6-dimethylbenzothiazolium chloride. E.g., a ZnO dispersion was made by mixing a butadiene-styrene binder (1680 g. of a 30% by weight toluene solution of a copolymer consisting of 30 parts by weight butadiene and 70 parts by weight styrene), toluene (1104 g.), and ZnO USP-12 (1915 g.) for 0.5 hr. in a 1-gal. Waring Blender at 107°F. After standing, the dispersion was filtered through coarse sintered glass filters. The ZnO dispersion (200 g.) was added to vessels containing varying amts. of sensitizing dyes. Coatings (1.5 mil dry thickness) of the sensitized dispersions in the vessels were placed on Al foil. After storing the vessels in the dark for 24 hrs., a 2nd set of photoconductor sheets was prepared by coating the dispersion again on Al foil. Color prints were made with a spectrograph at a 4 sec. exposure to the light source followed by a 10 sec. development at 30 v., with the application of the plating current. The areas of sensitivity of the photoconductor as evidenced by image development in the sensitized areas were shown to be significantly greater on those sheets treated with dispersion prepared with the chelating agent.

IT 13018-00-3 15637-36-2

RL: USSS (Uses)

(zinc oxide photoconductor supersensitization by)

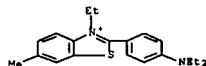
RN 13018-00-3 HCAPLUS

CN Benzothiazolium, 2-[p-(diethylamino)phenyl]-3-ethyl-6-methyl-, p-toluenesulfonate (8CI) (CA INDEX NAME)

CM 1

CRN 47290-32-4

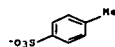
CMF C20 H25 N2 S



CM 2

CRN 16722-51-3

CMF C7 H7 O3 S



RN 15637-36-2 HCAPLUS

CN Benzothiazolium, 3-benzyl-2-[p-(dibenzylamino)phenyl]-6-methyl-, bromide (8CI) (CA INDEX NAME)

dimethylaminophenyl)benzimidazole, 161°; 1-methyl-2-(4-diethylaminophenyl)benzimidazole, 124°; 1-methyl-2-(4-hydroxyl-naphthyl)benzimidazole, 311°; 1-methyl-2-(4-dimethylaminophenyl)-6-methylbenzimidazole, 180°; 1-methyl-2-(3,4-methylenedioxyphenyl)-5-methylbenzimidazole, 149°; 1-methyl-2-(4-dimethylaminophenyl)-5-methylbenzimidazole, 161°; 1-methyl-2-(4-diethylaminophenyl)-5-methylbenzimidazole, 149°; 1-methyl-2-(4-methoxyphenyl)-5-nitrobenzimidazole, 171°; 1-methyl-2-(4-dimethylaminophenyl)-5-nitrobenzimidazole, 238°; 1-methyl-2-(4-diethylaminophenyl)-5-nitrobenzimidazole, 154°; 1-ethyl-2-(2-hydroxyphenyl)benzimidazole, 129°; 1-phenyl-2-(4-dimethylaminophenyl)benzimidazole, 222°; 1-phenyl-2-(4-diethylaminophenyl)benzimidazole, 148°; 1-(4-dimethylaminophenyl)-2-(2-hydroxyphenyl)-6-chlorobenzimidazole, 218°; 1-(4-dimethylaminophenyl)-2-(4-dimethylaminophenyl)-6-chlorobenzimidazole, 217°; 1-benzyl-2-(4-hydroxyphenyl)benzimidazole, 233°; 2-(p-dimethylaminophenyl)naphth[2t,3':4,5]imidazole, 300° (inters); 2-(2-pyridyl)naphthimidazole, 224-5°; 1-methyl-2-(2-hydroxyphenyl)naphth[4,5:1,2']imidazole, 155°; 1-ethyl-2-(4-dimethylaminophenyl)-7-methoxy[4,5:1,2']imidazole, 208°; 2-phenylphenanthro[9',10':4,5]oxazole, 200-2°; 2-(4-chlorophenyl)phenanthro[9',10':4,5]oxazole, 256-7°; 2-(4-methoxyphenyl)phenanthro[9',10':4,5]oxazole, 179-80°; 2-(4-diethylaminophenyl)phenanthro[9',10':4,5]oxazole, 260-5°; 2-furylphenanthro[9',10':4,5]oxazole, 228-30°; 1-methyl-2-(2-pyridyl)-5-methylbenzimidazole, 193°; 1-methyl-2-(2-pyridyl)-5-methylbenzimidazole, 114°; 2-(4-aminophenyl)benzimidazole, 240°; 2-(3-amino-4-dimethylaminophenyl)-6-methylbenzothiazole, 109°; 2-(3-nitro-4-dimethylaminophenyl)-6-methylbenzothiazole, 144°; 2-(4-dimethylaminophenyl)-6-methylbenzothiazole-sulfonamide, 244°; 2-(4-dimethylaminophenyl)-6-methylbenzothiazole-N-monomethylsulfonamide, 204°; the N-ethylsulfonamide (I), 172°; 2-(4-dimethylaminophenyl)-6-methylbenzothiazole-sulfonic acid morpholine, 189°; II, 202°; and III, 224°. An opaque paper base which was permeable to light rays and which had been treated to resist penetration of organic solvents was coated with .apprx. 6 μ thick coating by means of a solution made by dissolving 10 g. of a post-chlorinated poly(vinyl chloride) (having a Cl content of .apprx. 60%) in 100 g. MeCOEt, then adding 1cc a solution of 10 g. 2-(4'-dimethylaminophenyl)naphtho[2',3':4,5]imidazole in 50 g. toluene and then a solution of 0.01 g. Rhodamine B extra in 2 g. MeOH. The coated paper was given a neg. elec. charge and then placed with the coated side against a book page (printed on both sides and backed by black paper); a reflex image was produced by exposing to a 100-w. incandescent bulb through the paper for 1 sec. The image was developed by a developer powder consisting of 2.5 g. toner (30 parts Polystyrol LD, 30 parts Beckacite K 105, and 3 parts Peerless Black Russ 552) and 100 g. glass balls to yield a pos. reverse image. A non-reverse pos. image of the original was transferred to a second sheet by firmly pressing the sheet onto the powder image. Transfer can be aided by application of an elec. field to the second sheet in known manner.

IT 10205-57-9P, Benzothiazole, 2-[p-(diethylamino)phenyl]-

10205-63-7P, Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methyl-

10205-72-8P, Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methoxy-

10205-78-4P, Benzothiazole, 2-[p-(diethylamino)phenyl]-6-

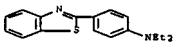
(dimethylamino)-

RL: PREP (Preparation)

(preparation of)

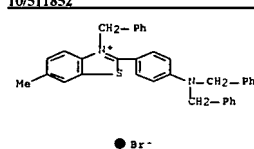
RN 10205-57-9 HCAPLUS

CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



RN 10205-63-7 HCAPLUS

CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



L21 ANSWER 54 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:508057 HCAPLUS Full-text

DOCUMENT NUMBER: 65:108057

ORIGINAL REFERENCE NO.: 65:20130d-h,2013a-e

TITLES: Organic photoconductive materials for electrophotography

INVENTOR(S): Suss, Oskar; Tomasek, Martha; Lind, Erwin

PATENT ASSIGNEE(S): Azoplate Corp.

SOURCE: 16 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

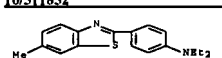
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3257204		19660621	US 1959-834680	19590819
			DE	19580822

PRIORITY APPLN. INFO.:

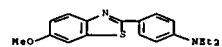
GI For diagram(s), see printed CA Issue.

AB Electrophotographic elements and processes utilizing polynuclear oxazole, thiazole, and imidazole compds. are reported. These are photoconductive and especially suited to production of very stable homogeneous layers. The compds. were prepared by known methods and are as follows (m.p. given): 2-phenylbenzothiazole, 114°; 2-(4-methoxyphenyl)benzothiazole, 134°; 2-(4-aminophenyl)benzothiazole, 157°; 2-(4-dimethylaminophenyl)benzothiazole, 173°; 2-(4-diethylaminophenyl)benzothiazole, 125°; 2-phenyl-6-methylbenzothiazole, 125°; 2-(4-methoxyphenyl)-6-methylbenzothiazole, 174°; 2-(4-aminophenyl)-6-methylbenzothiazole, 191°; 2-(4-acetylamino)phenyl-6-methylbenzothiazole, 225°; 2-(4-dimethylaminophenyl)-6-methylbenzothiazole, 196-7°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole, 128°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole N,N-dimethylsulfonamide, 145°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole N,N-diethyl-sulfonamide, 145°; 2-(3-methoxy-4-hydroxyphenyl)-6-methylbenzothiazole, 213°; 2-(3-hydroxy-4-methoxyphenyl)-6-methylbenzothiazole, 138°; 2-(2-methoxy-6-hydroxyphenyl)-6-methylbenzothiazole, 164°; 2-(3,4-dihydroxyphenyl)-6-methylbenzothiazole, 271°; 2-phenyl-6-methoxybenzothiazole, 117°; 2-(4-methoxyphenyl)-6-methoxybenzothiazole, 163°; 2-(4-dimethylaminophenyl)-6-methoxybenzothiazole, 182°; 2-(4-diethylaminophenyl)-6-methoxybenzothiazole, 140°; 2-phenyl-6-dimethyl-aminobenzothiazole, 133°; 2-(4-methoxyphenyl)-6-dimethyl-aminobenzothiazole, 151°; 2-(4-nitrophenyl)-6-diethylamino-benzothiazole, 246°; 2-(3-nitrophenyl)-6-dimethylaminobenzothiazole, 176°; 2-(2-nitrophenyl)-6-dimethylaminobenzothiazole, 147°; 2-(4-dimethylaminophenyl)-6-dimethylaminobenzothiazole, 230°; 2-(4-diethylaminophenyl)-6-dimethylaminobenzothiazole, 171°; 2-(3,4-methylenedioxyphenyl)-6-dimethylaminobenzothiazole, 176°; 2-phenylbenzoxazole, 102°; 2-(4-methoxyphenyl)benzoxazole, 99°; 2-(4-dimethoxyphenyl)benzoxazole, 182°; 2-(4-dimethylaminophenyl)benzoxazole, 132°; 2-(4-methoxyphenyl)-6-methylbenzoxazole, 91°; 2-(4-diethylaminophenyl)-6-methylbenzoxazole, 189°; 2-(4-diethylamino phenyl)-6-methylbenzoxazole, 108°; 2-(4-methoxyphenyl)-5-chlorobenzoxazole, 148°; 2-(4-dimethylaminophenyl)-5-chlorobenzoxazole, 179°; 2-(4-diethylaminophenyl)-5-chlorobenzoxazole, 160°; 2-(3-methoxy-4-hydroxyphenyl)benzimidazole, 222°; 2-(4-diethylaminophenyl)benzimidazole, 233°; 1-methyl-2-(3,4-methylenedioxyphenyl)benzimidazole, 160°; 1-methyl-2-(4-



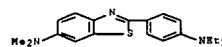
RN 10205-72-8 HCAPLUS

CN Benzenamine, N,N-diethyl-4-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 10205-78-4 HCAPLUS

CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 55 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:491193 HCAPLUS Full-text

DOCUMENT NUMBER: 65:91193

ORIGINAL REFERENCE NO.: 65:17102b-d

TITLES: Azo-substituted photographic color formers

INVENTOR(S): Pietrzok, Hubertus; Traue, Siegfried; Schmidt., Siegfried

SOURCE: 8 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 48302		19660605	DD	19650518
			DD	19650518

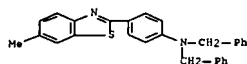
PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

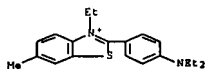
AB By coupling a naphthol or pyrazolone color former (for cyan and magenta images, resp.) with a diazotized 4'-amino-p-toluenesulfonamide (I) derivative, products are obtained which recouple readily in a color developer to give indoaniline or azomethine dyes with splitting off of the azo group, and which are stable in Ag bleach baths, especially at high pH. The color of the azo dye provides masking for undesired absorption of the main image dye. The color formers contain long-chain alkyl groups, rendering them nondiffusing, as well as solubilizing acid groups. Thus, I → 1,2-HOC10H6CONHC6H3(C18H37)MeSO3H-2,5 developed with 4-H2NOC6H4N2Et2, (II) forms blue-green images and provides a purple mask, while III gives a purple image with II and a yellow mask.

IT 10274-22-3P, Benzothiazole, 2-[p-(dibenzylamino)phenyl]-6-methyl-13018-00-3P, Benzothiazolium compounds, 2-[p-(diethylamino)phenyl]-3-ethyl-6-methyl-, p-toluenesulfonate 15637-36-2P.

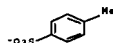
Benothiazolium compounds, 3-benzyl-2-[p-(dibenzylamino)phenyl]-6-methyl-, bromide  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 10274-22-3 HCAPLUS  
 CN Benothiazolium, 2-[p-(dibenzylamino)phenyl]-6-methyl- (7CI, 8CI) (CA INDEX NAME)



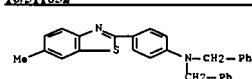
RN 13018-00-3 HCAPLUS  
 CN Benothiazolium, 2-[p-(diethylamino)phenyl]-3-ethyl-6-methyl-, p-toluenesulfonate (8CI) (CA INDEX NAME)  
 CM 1  
 CRN 47290-32-4  
 CMF C20 H25 N2 S



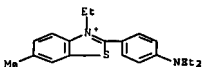
CM 2  
 CRN 16722-51-3  
 CMF C7 H7 O3 S



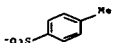
RN 15637-36-2 HCAPLUS  
 CN Benothiazolium, 3-benzyl-2-[p-(dibenzylamino)phenyl]-6-methyl-, bromide (8CI) (CA INDEX NAME)



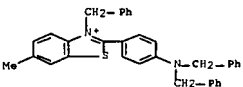
RN 13018-00-3 HCAPLUS  
 CN Benothiazolium, 2-[p-(diethylamino)phenyl]-3-ethyl-6-methyl-, p-toluenesulfonate (8CI) (CA INDEX NAME)  
 CM 1  
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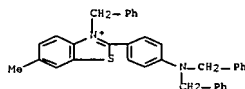
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 CRN 16722-51-3  
 CMF C7 H7 O3 S



RN 15637-36-2 HCAPLUS  
 CN Benothiazolium, 3-benzyl-2-[p-(dibenzylamino)phenyl]-6-methyl-, bromide (8CI) (CA INDEX NAME)



Br-



Br-

L21 ANSWER 56 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1966:491192 HCAPLUS Full-text  
 DOCUMENT NUMBER: 65:91192  
 ORIGINAL REFERENCE NO.: 65:17101f-g,17102a-b  
 TITLE: Compositions for use as photoconductors  
 PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co.  
 SOURCE: 5 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1037771		19660803	GB 1962-46815	19621211
			US	19611211

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

AB Dye-sensitized ZnO dispersions are supersensitized by adding compds. of the general formula I, and aging until the color of the I has disappeared. I are prepared by quaternization of II. Thus, a mixture of 252 g. ZnO, 151 g. PhMe, and 6 cc. 2% I (R = Me, X = Cl) (III) in MeOH was diluted with 26 g. PhMe and 20 g. MeOH treated with 210 g. Pliolite S-7, blended 15 min., treated with 6 cc. of a saturated MeOH solution of yellow dye S1334 Pina (IV), 6 cc. 1% MeOH solution of Alphasurine 20, and 0.6 cc. 1% methanolic Phloxine B, filtered, treated with 6 cc. IV, filtered, and coated on an Al sheet to give a panchromatic photoconductive sheet whose photosensitivity was significantly greater than that of a control not containing III. A mixture of dehydrothio-p-toluidine (II, R = H) 12, 4-MeC6H4SO3Rt (V) 22, and K2CO3 7.6 g. in 150 ml. o-C6H4Cl2 was stirred and refluxed 12 hrs., filtered, and diluted with 700 ml. C7H16 to precipitate a dark liquid, which was separated by decantation. The supernatant liquid was filtered and saturated with HCl, and the resulting precipitate separated, dispersed in 200 ml. H2O, and aqueous NH3 added to II (R = Et) give (VI). A mixture of 4.9 g. VI and 5 g. V was kept 45 min. at 150° and extracted with PhMe to leave I (R = Et, X = 4-MeC6H4SO3), m. 142-4° (CSHSN-C7H14). Similarly, II (R = H) was benzylated to give II (R = CH2Ph), m. 192-5° (CSHSN-MeOH) which was quaternized to I (R = CH2Ph, X = Br), m. 161-3° I (R = Me) treated with 4-MeC6H4SO3Me gave I (R = Me, X = 4-MeC6H4SO3), m. 211-17° (CSHSN).

IT 10274-22-3, Benothiazolium, 2-[p-(dibenzylamino)phenyl]-6-methyl-13018-00-3P, Benothiazolium, 2-[p-(diethylamino)phenyl]-3-ethyl-6-methyl-, p-toluenesulfonate 15637-36-2P, Benothiazolium, 3-benzyl-2-[p-(dibenzylamino)phenyl]-6-methyl-, bromide  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 10274-22-3 HCAPLUS  
 CN Benothiazolium, 2-[p-(dibenzylamino)phenyl]-6-methyl- (7CI, 8CI) (CA INDEX NAME)

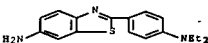
ACCESSION NUMBER: 1966:32500 HCAPLUS Full-text  
 DOCUMENT NUMBER: 64:32500  
 ORIGINAL REFERENCE NO.: 64:5996b-d  
 TITLE: Photoconductors for electrophotography  
 PATENT ASSIGNEE(S): Renker-Belipa G.m.b.H.  
 SOURCE: 21 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1008632		19651103	GB 1961-35562	19611002
DE 1216690			DE	19601003

PRIORITY APPLN. INFO.:

AB It has been assumed that organic photoconductors used to produce electrophotographic layers have to be used in the presence of insulating binders, the purpose of the latter being, at the least, to prevent discharge of the unexposed layer. It has now been found that photoconductors with per se binding properties are equally suitable. Such compds. contain groups with photoconductive properties along with groups to confer adhesive properties and are prepared by reaction of photoconductors carrying reactive groups with one or more compds. with epoxy and/or isocyanate groups with the further possible addition of cross-linking agents. Thus, 50 g. 2-(4'-aminophenyl)-6-methylbenzothiazole (m. 192°) dissolved in 750 ml. anhydrous cyclohexanone was mixed with 87.5 g. of 75% EtOAc solution of a modified tri-isocyanate (Desmodur L), and after distillation of the EtOAc, the mixture was refluxed for 30 min., cooled, and filtered. The precipitate was boiled with 500 ml. Me2CO, filtered hot, washed with more cold solvent, and dried at 100° to give an almost colorless product softening 220-5°. It was dissolved (100 g.) in 500 ml. cyclohexanone and 200 ml. EtOAc and coated onto an Al plate, which was then charged to 6-7 kv., exposed, dusted with a toner mixture, and heated to give an image of high resolution and good contrast.

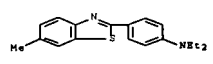
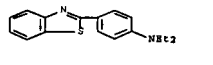
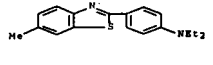
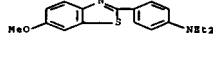
IT 5809-18-7, Benothiazole, 6-amino-2-[p-(diethylamino)phenyl]- (reaction product with epoxy resins, as photoconductor for electrophotography)  
 RN 5809-18-7 HCAPLUS  
 CN Benothiazole, 6-amino-2-[p-(diethylamino)phenyl]- (7CI, 8CI) (CA INDEX NAME)

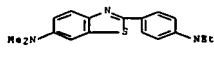


L21 ANSWER 58 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1963:462387 HCAPLUS Full-text  
 DOCUMENT NUMBER: 59:42387  
 ORIGINAL REFERENCE NO.: 59:11515b-h,11516a-c  
 TITLE: Materials for electrophotographic reproduction  
 INVENTOR(S): Sues, Oskar; Tomanek, Martha; Lind, Erwin  
 PATENT ASSIGNEE(S): Kalle A.-G.  
 SOURCE: 17 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

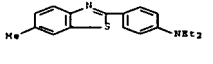
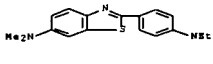
10/511852 185/217 Robert Havlin  
DS 1137625 19621004 DE 1958-KJ5586 19580822  
PRIORITY APPLN. INFO.: DE 19580822  
OI For diagram(s), see printed CA issue.  
AB Insulated layers formed from mixtures of organic colloids and photo-conductive thiazole, oxazole, or imidazole compds. 2-(4-acetaminophenyl)-6-methylbenzothiazole (I), 1 g. "Zinkresinat 357," and 0.02 g. Acid Violet 6 BN is dissolved in 30 g. glycol monomethyl ether, coated on paper, and dried. After undergoing a corona discharge, the sensitized paper is exposed under a pos. copy to a 100-w. incandescent bulb for 1/4 sec., dusted with a carbon-colored resin powder and fixed by heating. The substances used are of the formula I where X is a noncondensed aromatic ring, Y is a univalent aromatic or heterocyclic radical, Z is an O or S atom or an imino group in which the H atom is displaced by an alkyl or aralkyl radical. The following new compds. were prepared by known methods [compound and m.p. given]: 2-phenylbenzothiazole, 114°; 2-(4-methoxyphenyl)benzothiazole, 134°; 2-(4-aminophenyl)benzothiazole, 125°; 2-(4-diethylaminophenyl)benzothiazole, 173°; 2-(4-diethylaminophenyl)benzothiazole, 125°; 2-(4-methoxyphenyl)-6-methylbenzothiazole, 174°; 2-phenyl-6-methylbenzothiazole, 125°; 2-(4-aminophenyl)-6-methylbenzothiazole, 191°; 2-(4-acetaminophenyl)-6-methylbenzothiazole, 225°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole, 196-7°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole, 128°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole-N,N-dimethylsulfonamide, 145°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole-N,N-diethylsulfonamide, 145°; 2-(3-methoxy-4-hydroxyphenyl)-6-methylbenzothiazole, 213°; 2-(3-hydroxy-4-methoxyphenyl)-6-methylbenzothiazole, 138°; 2-(2-methoxy-6-hydroxyphenyl)-6-methylbenzothiazole, 164°; 2-(3,4-dihydroxyphenyl)-6-methylbenzothiazole, 271°; 2-(4-methoxyphenyl)-6-methoxybenzothiazole, 163°; 2-(4-diethylaminophenyl)-6-methoxybenzothiazole, 140°; 2-phenyl-6-methoxybenzothiazole, 117°; 2-(4-diethylaminophenyl)-6-methoxybenzothiazole, 182°; 2-phenyl-6-methylaminobenzo-1,3,5-triazole, 135°; 2-(4-nitrophenyl)-6-di-methylaminobenzo-1,3,5-triazole, 246°; 2-(3-nitrophenyl)-6-diethylaminobenzo-1,3,5-triazole, 176°; 2-(2-nitrophenyl)-6-diethylaminobenzo-1,3,5-triazole, 147°; 2-(4-diethylaminophenyl)-6-diethylaminobenzo-1,3,5-triazole, 230°; 2-(4-methoxyphenyl)-6-diethylaminobenzo-1,3,5-triazole, 151°; 2-(4-diethylaminophenyl)-6-diethylaminobenzo-1,3,5-triazole, 171°; 2-(3,4-methylenedioxyphenyl)-6-diethylaminobenzo-1,3,5-triazole, 176°; 2-phenylbenzoxazole, 102°; 2-(4-methoxyphenyl)benzoxazole, 99°; 2-(4-diethylaminophenyl)benzoxazole, 182°; 2-(4-diethylaminophenyl)benzoxazole, 132°; 2-(4-methoxyphenyl)-6-methylbenzoxazole, 91°; 2-(4-diethylaminophenyl)-6-methylbenzoxazole, 189°; 2-(4-diethylaminophenyl)-6-methylbenzoxazole, 108°; 2-(4-methoxyphenyl)-5-chlorobenzoxazole, 148°; 2-(4-diethylaminophenyl)-5-chlorobenzoxazole, 179°; 2-(4-diethylaminophenyl)-5-chlorobenzoxazole, 160°; 2-(3-methoxy-4-hydroxyphenyl)benzimidazole, 222°; 2-(4-diethylaminophenyl)benzimidazole, 233°; 1-methyl-2-(3,4-methylenedioxyphenyl)benzimidazole, 160°; 1-methyl-2-(4-diethylaminophenyl)benzimidazole, 161°; 1-methyl-2-(4-diethylaminophenyl)benzimidazole, 124°; 1-methyl-2-(4-hydroxy-1-naphthyl)benzimidazole, 311°; 1-methyl-2-(4-diethylaminophenyl)-6-methylbenzimidazole, 180°; 1-methyl-2-(3,4-methylenedioxyphenyl)-5-methylbenzimidazole, 149°; 1-methyl-2-(4-diethylaminophenyl)-5-methylbenzimidazole, 161°; 1-methyl-2-(4-diethylaminophenyl)-5-methylbenzimidazole, 149°; 1-methyl-2-(4-methoxyphenyl)-5-nitrobenzimidazole, 171°; 1-methyl-2-(4-diethylaminophenyl)-5-nitrobenzimidazole, 238°; 1-methyl-2-(4-diethylaminophenyl)-5-nitrobenzimidazole, 154°; 1-ethyl-2-(2-hydroxyphenyl)benzimidazole, 129°; 1-phenyl-2-(4-diethylaminophenyl)benzimidazole, 222°; 1-phenyl-2-(4-diethylaminophenyl)benzimidazole, 148°; 1-(4-diethylaminophenyl)-2-(2-hydroxyphenyl)-6-chlorobenzimidazole, 218°; 1-(4-diethylaminophenyl)-2-(4-diethylaminophenyl)-6-chlorobenzimidazole, 217°; 1-benzyl-2-(4-hydroxyphenyl)benzimidazole, 213°; 2-(p-diethylaminophenyl)naphth-[2',3',4,5]imidazole, 300° (decomposition); 2-(2-pyridyl)naphth-[2',3',4,5]imidazole, 224-5°; 1-methyl-2-(2-hydroxyphenyl)naphth-[4,5,1',2']imidazole, 155°; 1-ethyl-2-(4-diethylaminophenyl)-7-methoxynaphth-[4,5,1',2']imidazole, 208°; 2-phenylphenanthrene-[9',10',4,5]oxazole, 200-2°; 2-(4-chlorophenyl)phenanthrene-[9',10',4,5]oxazole, 256-7°; 2-(4-methoxyphenyl)phenanthrene-[9',10',4,5]oxazole, 179-180°; 2-(4-diethylaminophenyl)phenanthrene-[9',10',4,5]oxazole, 260-5°; 2-furylphenanthrene-[9',10',4,5]oxazole, 228-30°; 1-methyl-2-(2-pyrryl)-5-methylbenzimidazole, 193°; 1-methyl-2-(1-naphthyl)-5-methylbenzimidazole, 114°; 2-(4-aminophenyl)benzimidazole 240°; 2-(3-amino-4-diethylaminophenyl)-6-methylbenzothiazole, 109°; 2-(3-nitro-4-diethylaminophenyl)-6-methylbenzothiazole, 144°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole sulfamoyl derivative, 244°; 2-(4-

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dimethylaminophenyl)-6-methylbenzothiazole-N-methylsulfamoyl derivative, 204°; 2-(4-dimethylaminophenyl)-6-methylbenzothiazole-sulfonic acid morpholide, 189°. Also prepared were 11, m. 224, and the SO<sub>2</sub>NH<sub>2</sub> derivative of 111, m. 172°, yellow.  
IT 10205-63-7 HCAPLUS Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methyl- (dimethylamino) (diethylamino) derivative  
RN 10205-63-7 HCAPLUS Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methyl- (diethylamino) derivative  
CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
  
IT (dimethylsulfamoyl deriv. 10205-57-9P, Benzothiazole, 2-[p-(diethylamino)phenyl]- 10205-63-7P, Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methyl- 10205-72-6P, Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methoxy- 10205-78-4P, Benzothiazole, 2-[p-(diethylamino)phenyl]-6- (dimethylamino) - RL: PREP (Preparation) (preparation of) 10205-63-7 HCAPLUS  
RN 10205-63-7 HCAPLUS Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
  
RN 10205-63-7 HCAPLUS Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
  
RN 10205-72-8 HCAPLUS Benzenamine, N,N-diethyl-4-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
CN Benzenamine, N,N-diethyl-4-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
  
RN 10205-78-4 HCAPLUS 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)  
CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

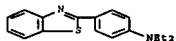
10/511852 187/217 Robert Havlin  
INDEX NAME  
  
L21 ANSWER 59 OF 64 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1962:473383 HCAPLUS Full-text  
DOCUMENT NUMBER: 57:73383  
ORIGINAL REFERENCE NO.: 57:14577g-1,14578a-1,14579a  
TITLE: Photoconductive substances for electrophotography  
PATENT ASSIGNER(S): Kalle & Co., A.-G.  
SOURCE: 11 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 895001		19620426	GB 1959-27912	19590814
			DE 19580822	19580822

PRIORITY APPLN. INFO.:  
AB Photoconductive insulating layers for electrophotog. are prepared by incorporation (from organic solvents), optionally with other photoconductive substances (and/or certain natural or synthetic resins, polymers or organic colloids), of thiazole, oxazole, or imidazole compds. Suitable compds. are (m.p. given): 2-phenylbenzothiazole, 114°; 2-(4-methoxyphenyl)benzothiazole, 134°; 2-(4-aminophenyl)benzothiazole, 125°; 2-(4-diethylaminophenyl)benzothiazole, 173° (alc.); 2-(4-diethylaminophenyl)benzothiazole, 125° (alc.); 2-phenyl-6-methylbenzothiazole, 125°; 2-(4-methoxyphenyl)-6-methylbenzothiazole, 174° (alc.); 2-(4-aminophenyl)-6-methylbenzothiazole (II), 191°; 2-(4-acetaminophenyl)-6-methylbenzothiazole, 225°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole, 196-7°; 2-(4-diethylaminophenyl)-6-methylbenzothiazole, 128° (alc.); 2-(4-diethylaminophenyl)-6-methyl- X-dimethylsulfamoylbenzothiazole (II), 145° (alc.); the diethylsulfamoyl analog of II, 145° (alc.); 2-(3-methoxy-4-hydroxyphenyl)-6-methylbenzothiazole, 213° (alc.); 2-(3-hydroxy-4-methoxyphenyl)-6-methylbenzothiazole, 138° (alc.); 2-(2-methoxy-6-hydroxyphenyl)-6-methylbenzothiazole, 164° (alc.); 2-(3,4-dihydroxyphenyl)-6-methylbenzothiazole, 271° (alc.); 2-(4-methoxyphenyl)-6-methoxybenzothiazole, 140° (alc.); 2-phenyl-6-methoxybenzothiazole, 117°; 2-(4-methoxyphenyl)-6-methoxybenzothiazole, 163° (alc.); 2-(4-diethylaminophenyl)-6-methoxybenzothiazole, 182°; 2-(4-diethylaminophenyl)-6-methoxybenzothiazole, 140° (alc.); 2-phenyl-6-methylaminobenzo-1,3,5-triazole, 135°; 2-(4-diethylaminophenyl)-6-methylaminobenzo-1,3,5-triazole, 151° (alc.); 2-(4-nitrophenyl)-6-methylaminobenzo-1,3,5-triazole, 246°; 2-(3-nitrophenyl)-6-methylaminobenzo-1,3,5-triazole, 176°; 2-(2-nitrophenyl)-6-methylaminobenzo-1,3,5-triazole, 147°; 2-(4-diethylaminophenyl)-6-methylaminobenzo-1,3,5-triazole, 230°; 2-(4-diethylaminophenyl)-6-methylaminobenzo-1,3,5-triazole, 171° (alc.); 2-(3,4-methylenedioxyphenyl)-6-methylaminobenzo-1,3,5-triazole, 176° (alc.); 2-phenylbenzoxazole, 102°; 2-(4-methoxyphenyl)benzoxazole, 99°; 2-(4-diethylaminophenyl)benzoxazole, 182°; 2-(4-diethylaminophenyl)benzoxazole, 132° (alc.); 2-(4-methoxyphenyl)-6-methylbenzoxazole, 91° (alc.); 2-(4-diethylaminophenyl)-6-methylbenzoxazole, 189° (alc.); 2-(4-diethylaminophenyl)-6-methylbenzoxazole, 108°; 2-(4-diethylaminophenyl)-5-chlorobenzoxazole, 148°; 2-(4-diethylaminophenyl)-5-chlorobenzoxazole, 179°; 2-(4-diethylaminophenyl)-5-chlorobenzoxazole, 160° (C6H6/light petroleum); 2-(3-methoxy-4-hydroxyphenyl)benzimidazole, 222°; 2-(4-diethylaminophenyl)benzimidazole, 233°; 1-methyl-2-(3,4-methylenedioxyphenyl)benzimidazole, 160° (alc.); 1-methyl-2-(4-diethylaminophenyl)benzimidazole, 161° (C6H6/light petroleum); 1-methyl-2-(4-diethylaminophenyl)benzimidazole, 124° (light petroleum); 1-methyl-2-(4-hydroxy-1-naphthyl)benzimidazole, 311° (alc.); 1-methyl-2-(4-diethylaminophenyl)-6-methylbenzimidazole, 180° (C6H6/light petroleum); 1-methyl-2-(3,4-methylenedioxyphenyl)-5-methylbenzimidazole, 149° (50% aqueous alc.); 1-methyl-2-(4-diethylaminophenyl)-5-methylbenzimidazole, 161° (50% aqueous alc.); 1-methyl-2-(4-diethylaminophenyl)-5-

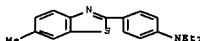
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methylbenzimidazole, 149° (50% aqueous alc.); 1-methyl-2-(4-methoxyphenyl)-5-nitrobenzimidazole, 171° (alc.); 1-methyl-2-(4-diethylaminophenyl)-5-nitrobenzimidazole, 238° (alc.); 1-methyl-2-(4-diethylaminophenyl)-5-nitrobenzimidazole, 154° (alc.); 1-ethyl-2-(2-hydroxyphenyl)benzimidazole, 129° (alc.); 1-phenyl-2-(4-diethylaminophenyl)benzimidazole, 222° (alc.); 1-phenyl-2-(4-diethylaminophenyl)benzimidazole, 148° (aqueous MeOH); 1-(4-diethylaminophenyl)-2-(2-hydroxyphenyl)-6-chlorobenzimidazole, 218° (dioxane); 1-(4-diethylaminophenyl)-2-(4-diethylaminophenyl)-6-chlorobenzimidazole, 217° (alc.); 1-benzyl-2-(4-hydroxyphenyl)benzimidazole, 233° (dioxane); 2-(4-diethylaminophenyl)naphth-[2',3',4,5]imidazole, sinter from 300°; 2-(2-pyridyl)naphthimidazole, 224-5° (alc.); 1-methyl-2-(2-hydroxyphenyl)naphth-[4,5,1',2']imidazole, 155° (alc.); 1-ethyl-2-(4-diethylaminophenyl)-7-methoxynaphth-[4,5,1',2']imidazole, 208° (C6H6/light petroleum); 2-phenylphenanthrene-[9',10',4,5]oxazole, 200-2°; 2-(4-chlorophenyl)phenanthrene-[9',10',4,5]oxazole, 256-7° (dioxane); 2-(4-methoxyphenyl)phenanthrene-[9',10',4,5]oxazole, 179-80° (80% EtOH); 2-(4-diethylaminophenyl)phenanthrene-[9',10',4,5]oxazole, 260-5° (96% alc.); 2-(2-furyl)phenanthrene-[9',10',4,5]oxazole, 228-30° (dioxane); 1-methyl-2-(2-pyrryl)-5-methylbenzimidazole, 193° (alc.); 1-methyl-2-(1-naphthyl)-5-methylbenzimidazole, 114° (light petroleum); 2-(4-aminophenyl)benzimidazole, 240°; 2-(4-phenylureido)phenyl)-6-methylbenzothiazole, 202° (Me<sub>2</sub>CO); 2-(3-amino-4-diethylaminophenyl)-6-methylbenzothiazole, 109° (MeOH); 2-(3-nitro-4-diethylaminophenyl)-6-methylbenzothiazole, 144° (alc.); 2-(3-phenylureido-4-diethylaminophenyl)-6-methylbenzothiazole, 224° (Me<sub>2</sub>CO); 2-(4-diethylaminophenyl)-6-methyl-γ-benzothiazole-sulfonamide, 244° (HOC(CH<sub>2</sub>)<sub>2</sub>CH<sub>2</sub>OH); 2-(4-diethylaminophenyl)-6-methyl-N-methyl-γ-benzothiazole-N-sulfonamide, m. 204° (alc.); 2-(4-diethylaminophenyl)-6-methyl-N-ethyl-γ-benzothiazole-sulfonamide, 178° (75% alc.); 2-(4-diethylaminophenyl)-6-methyl-γ-benzothiazole-sulfonic acid morpholide, 189° (alc.). The spectral sensitivity of photoconducting insulating layers can be extended into the visible by addition (1-3% based on the weight of photoconductive substance) of chlorophyll or certain triarylmethane, xanthene, thiazine, acridine, or cyanine dyes, phthalene, or quinone and ketone dyes. Thus, to a solution of 10 g. chlorinated poly(vinyl chloride) in 100 g. MeCOEt, 10 g. I in 50 g. PhMe and 0.004 g. ethyl violet in 2 g. MeOH were added. A 6 μ thick coating was prepared and after drying pos. charged with a corona discharge. After episcopically producing a latent image from a printed page, a developer (resin coating and finely divided mixture of resin and carbon black fused to tiny glass balls) was applied. Adherence of the pigmented resin to the non-exposed areas was then made permanent by light heating.  
IT 10205-63-7 HCAPLUS Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methyl- 10205-78-4 HCAPLUS Benzothiazole, 2-[p-(diethylamino)phenyl]-6- (dimethylamino) - (as photoconductor for electrophotog.)  
RN 10205-63-7 HCAPLUS Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)  
  
RN 10205-78-4 HCAPLUS 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)  
CN 6-Benzothiazolamine, 2-[4-(diethylamino)phenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)  


L21 ANSWER 60 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1958:73571 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 52:73571  
 ORIGINAL REFERENCE NO.: 52:13094f-h  
 TITLE: Tuberculostatic activity of certain 2-phenylbenzothiazole derivatives  
 AUTHOR(S): Prescott, Benjamin; Webb, Junius M.  
 CORPORATE SOURCE: Natl. Insts. of Health, Bethesda, MD  
 SOURCE: Antibiotics and Chemotherapy (Washington, D. C.) (1958), 8, 33-6  
 CODEN: ANTCAG; ISSN: 0570-3123  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB Thirty-six 2-phenylbenzothiazole deriva. were prepared and tested for acute toxicity in mice and in vitro activity with avirulent Mycobacterium tuberculosis. The deriva. were prepared by condensation of 2-aminobenzeneethiol with various aromatic aldehydes in 95% EtOH at room temperature or by refluxing 30 min. on a steam bath and crystallizing the insol. products from 95% EtOH. The m.p. of certain deriva. is given: 2-(2-ethoxyphenyl) (I) 66, 2-(2,3-dimethoxyphenyl) (II) 60, 2-(2-methoxyphenyl) (III) 92, 2-phenyl 104, 2-(4-hydroxyphenyl) 226, 2-(4-diethylaminophenyl) 107, 2-(4-methoxyphenyl) 115, 2-(3-ethoxy-4-hydroxyphenyl) 120, 2-(4-dimethylaminophenyl) 148, 2-(2-nitrophenyl) 115, 2-(2,4-dihydroxyphenyl) 77. I, II, III, and 2-(2-hydroxy-5-nitrophenyl)benzothiazole inhibited M. tuberculosis at 2.5-5  $\mu$ M., as did isoniazid. They were less toxic to mice, which tolerated intraperitoneal injections of 1000-8000 mg./Kg., than isoniazid which was acutely toxic at 100 mg./kg.  
 IT 10205-57-9, Benzothiazole, 2-(p-diethylaminophenyl)- (Mycobacterium tuberculosis inhibition by)  
 RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

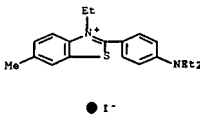


L21 ANSWER 61 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1957:43302 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 51:43302  
 ORIGINAL REFERENCE NO.: 51:80711,8072a-f  
 TITLE: Steric hindrance in quaternary salts of 2-arylbenzothiazoles and 2-arylbenzoselezenazoles  
 AUTHOR(S): Kiprianov, A. I.; Shrubovich, V. A.  
 CORPORATE SOURCE: State Univ., Kiev  
 SOURCE: Zhurnal Obshchei Khimii (1956), 26, 2591-6  
 CODEN: ZOKH44; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The absorption maxima of sulfates of 2-p-dimethylaminophenyl deriva. of benzothiazole, 6-methylbenzothiazole,  $\alpha$ -naphthothiazole, and benzoselezenazole in EtOH are displaced to longer wavelengths in comparison with quaternary salts of these substances. This unusual phenomenon indicates the quaternary salts of coplanarity of benzenoid and thiazole or selenazole rings in the quaternary salts owing to steric hindrance. Heating 7.2 g. o-H2NC6H4SeH and 8.3 g. p-Me2NC6H4CHO 3 hrs. at 100° gave 2-p-dimethylaminophenylbenzothiazole, m. 172°,  $\lambda$  362 m $\mu$ ; methiodide, decompose 220°,  $\lambda$  420 m $\mu$ ; ethiodide, m. 176°,  $\lambda$  423 m $\mu$ . 6-Methyl-2-p-

diethylaminophenylbenzothiazole (cf. Hunter, C.A. 18, 984), m. 116°,  $\lambda$  364 m $\mu$ ; ethiodide, m. 140°,  $\lambda$  427 m $\mu$ . The crude chloride (6 g.) from 2-ClOH7NH2.HCl and S2Cl2 in AcOH (Zubarovskii, C.A. 42, 906b) refluxed with 4 g. KOH in EtOH, then treated with 3.6 g. p-Me2NC6H4CHO and refluxed 1.5 hrs. gave 0.63 g. yellowish 2-p-dimethylaminophenyl- $\alpha$ -naphthothiazole, m. 174°,  $\lambda$  370 m $\mu$ ; ethiodide, m. 165-6°,  $\lambda$  430 m $\mu$ . Zn salt of o-H2NC6H3SeH (4.4 g.) and 3.2 g. p-Me2NC6H4CHO in 2 ml. concentrated HCl heated 1 hr. at 100° and 10 min. at 130°, then treated with NaOH, followed by HCl, and chromatographed on Al2O3 with elution by CHCl3 gave 1 g. 2-p-dimethylaminophenylbenzoselezenazole, m. 178°,  $\lambda$  364 m $\mu$ ; ethoperchlorate, decompose 170°,  $\lambda$  430 m $\mu$ . 2-p-Dimethylaminophenylbenzoxazole, m. 182-3°,  $\lambda$  295 m $\mu$ , heated with p-Me2NC6H4SO3Et gave [4-(2-benzoxazolyl)phenyl]dimethylethylammonium tosylate, m. 190-1°,  $\lambda$  300 m $\mu$ . p-Me2NC6H4CO2H failed to form the anhydride by the directions of Decombe (C.A. 46, 1508a), yielding only high melting substances; however pure K salt of the acid (5 g.) suspended in chilled C6H6 and treated with cooling with 3.1 g. (COCl)2, stirred 0.5 hr., and heated 0.5 hr. to reflux gave after separation of KCl and concentration 50% p-dimethylaminobenzoyl chloride, m. 147-8°, which heated with o-H2NC6H4OH 10 min. to 180° gave after extraction with hot EtOH a residue of p-dimethylaminophenylbenzoxazole, while the solution with NaClO4 gave 2-p-dimethylaminophenylbenzoxazole etherperchlorate, m. 226-7°,  $\lambda$  400 m $\mu$ . 2-p-Dimethylaminostyrylbenzothiazole, m. 206-8°,  $\lambda$  400 m $\mu$ ; ethiodide, decompose 237°,  $\lambda$  530 m $\mu$ . Heating 1.11 g. p-Me2NC6H4CHO and 0.22 ml. concentrated HCl 8 hrs. to 100° and 3.5 hrs. to 130°, with 1.5 g. 2-methyl- $\alpha$ -naphthothiazole gave after treatment with NaOH 32% yellow 2-p-dimethylaminostyryl- $\alpha$ -naphthothiazole, m. 220°,  $\lambda$  370 m $\mu$ ; ethiodide,  $\lambda$  537 m $\mu$ . Condensation of 2-methylbenzoselezenazole with p-Me2NC6H4CHO with HCl gave 2-p-dimethylaminostyrylbenzoselezenazole, m. 198°,  $\lambda$  403 m $\mu$ ; ethiodide, decompose 237°,  $\lambda$  537 m $\mu$ . Condensation of 2-methylbenzoxazole with p-Me2NC6H4CHO gave 2-p-dimethylaminostyrylbenzoxazole, m. 174°,  $\lambda$  394 m $\mu$ ; methiodide, m. 220°,  $\lambda$  495 m $\mu$ .  
 IT 10205-63-7, Benzothiazole, 2-(p-diethylaminophenyl)-6-methyl-111065-80-6, 2-(p-Diethylaminophenyl)-3-ethyl-6-methylbenzothiazolium iodide (and its spectrum)  
 RN 10205-63-7 HCAPLUS  
 CN Benzenamine, N,N-diethyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



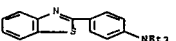
RN 111065-80-6 HCAPLUS  
 CN 2-(p-Diethylaminophenyl)-3-ethyl-6-methylbenzothiazolium iodide (6CI) (CA INDEX NAME)



L21 ANSWER 62 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1956:40624 HCAPLUS  
 DOCUMENT NUMBER: 50:40624  
 ORIGINAL REFERENCE NO.: 50:7872a-e  
 TITLE: Sulfonic acid derivatives of 2-(4'-dialkylaminophenyl)-benzothiazole  
 INVENTOR(S): Zwilgmeyer, Frithjof  
 PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

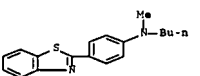
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2715629		19550816	US 1952-299260	19520716

AB 2-(4'-Dialkylaminophenyl)benzothiazoles (I), with alkyl groups of 5-6 C atoms, are sulfonated to monosulfonic acids with excellent fluorescent power of proper bluish hue for whitening paper. Sulfonation is effected with oleum at 40-60°, followed by neutralization with Na, K, or NaOH, and recovery of the corresponding sulfonate. E.g., 2-(4'-dimethylaminophenyl)benzothiazole (II) 30 added to 25% oleum 1000 parts with agitation at room temperature until it dissolved, the solution heated to 50° and kept at this temperature until a sample dissolved to a clear solution in dilute aqueous NaOH or Na2CO3 (which required about 1 hr.), the mass then drowned in ice water, filtered, the filter cake (the free monosulfonic acid derivative of II) washed nearly acid-free with ice water and added to 100 parts water, the mixture neutralized with NaOH at 85-90°, 15 parts NaCl added, the mixture cooled to 20° and agitated at this temperature until the mono(sodium sulfonate) crystallized out, and the product filtered, washed with 15% NaCl solution, and dried gave the mono(sodium sulfonate) of II in good yield. Similarly, the following I (alkylamino group given) were monosulfonated and converted into their Na salts: MeEtN, Et2N, Pr2N, Bu2N, and MeBu. To 1000 parts bleached sulfite wood pulp (air-dry basis) suspended in 20,000 parts water in a paper beater machine at 20-30° is added 1 part mono(sodium sulfonate) of II in 100 parts water, the mixture circulated 15 min., 20 parts standard saponified rosin size and 25 parts Al2(SO4)3.18H2O are added, the beating is continued 30 min., and the mixture diluted with 180,000 parts water, and formed into a sheet. The paper thus obtained possesses a brilliant blue fluorescence when viewed in ultraviolet light; in ordinary daylight it is much brighter and whiter than untreated paper. For surface application 0.5% is dissolved in a 5% starch solution  
 IT 10205-57-9, Benzothiazole, 2-(p-diethylaminophenyl)-  
 778533-33-8, Benzothiazole, 2-(p-dibutylaminophenyl)-  
 854058-76-7, Benzothiazole, 2-(p-(butylmethylamino)phenyl)-  
 854070-78-3, Benzothiazole, 2-(p-dipropylaminophenyl)-  
 854085-25-9, Benzothiazole, 2-[p-(ethylmethylamino)phenyl]- (sulfo derivative, and its Na salt)  
 RN 10205-57-9 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-dibutyl- (9CI) (CA INDEX NAME)

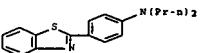


RN 778533-33-8 HCAPLUS  
 CN Benzenamine, 4-(2-benzothiazolyl)-N,N-dibutyl- (9CI) (CA INDEX NAME)

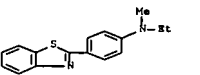
RN 854058-76-7 HCAPLUS  
 CN Benzothiazole, 2-[p-(butylmethylamino)phenyl]- (5CI) (CA INDEX NAME)



RN 854070-78-3 HCAPLUS  
 CN Benzothiazole, 2-(p-dipropylaminophenyl)- (5CI) (CA INDEX NAME)



RN 854085-25-9 HCAPLUS  
 CN Benzothiazole, 2-[p-(ethylmethylamino)phenyl]- (5CI) (CA INDEX NAME)



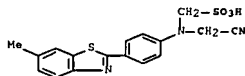
L21 ANSWER 63 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1955:19977 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 49:19977  
 ORIGINAL REFERENCE NO.: 49:3915c-d  
 TITLE: Syntheses of organic fluorescent compounds. XIX. Syntheses of fluorescent compounds by means of cyanomethylation and their optical bleaching effect  
 AUTHOR(S): Oda, Ryohel; Yoshida, Zenichi; Shimada, Yukiyasu  
 CORPORATE SOURCE: Kyoto Univ.  
 SOURCE: Kogyo Kagaku Zasshi (1952), 55, 786-7  
 CODEN: KOKZ7A; ISSN: 0368-5462  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB 1-ClOH7N(CH2CN)CH2SO3H, 6-methyl-2-[4-[N-(cyanomethyl)sulfomethylamino]phenyl]benzothiazole, and 2-(cyanomethylamino)-2'-(sulfomethylamino)-stilbene have strong

intensities of violet to blue fluorescence in the solid state and have good solubility with high optical bleaching effect on wool (except the 1st compound) and light fastness.

IT 855455-04-2, Benzothiazole, 2-[p-[(cyanomethyl)(sulfomethyl)amino]phenyl]-6-methyl-, sodium salt (fluorescence of)

RN 855465-04-2 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED



● Na

L21 ANSWER 64 OF 64 HCAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1955:19975 HCAPLUS Full-text

DOCUMENT NUMBER: 49:19975

ORIGINAL REFERENCE NO.: 49:39141,3915a-b

TITLE: Syntheses of organic fluorescent compounds. XVII.

Syntheses of water-soluble fluorescent compounds by

means of sulfomethylation of monoamino compounds and

their optical bleaching effect

Oda, Ryohei; Yoshida, Zenichi; Shimada, Yukiyasu

Kyoto Univ.

Kogyo Kagaku Zasshi (1952), 55, 782-4

CODEN: KOKZAT; ISSN: 0368-5462

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

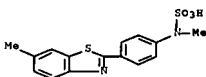
AB of. C.A. 49, 1700e. The formation of RCH<sub>2</sub>SO<sub>3</sub>Na from RNH<sub>2</sub>, CH<sub>2</sub>O, and NaHSO<sub>3</sub> is termed sulfomethylation. The measurements of fluorescence intensities of 1- and 2-H<sub>2</sub>NClO<sub>6</sub>NHCH<sub>2</sub>SO<sub>3</sub>Na, Na (1-carbazolylamino)methanesulfonate, 6-methyl-2-[4-(sulfomethylamino)phenyl]benzothiazole, etc., revealed that the compds. in solid state have strong or medium intensities of violet or bluish violet fluorescence. The optical bleaching effect was recognized for wool in the last compound above mentioned.

IT 854072-23-4, Benzothiazole, 6-methyl-2-[p-(sulfomethylamino)phenyl]-, sodium salt (fluorescence of)

RN 854072-23-4 HCAPLUS

CN Benzothiazole, 6-methyl-2-[p-(sulfomethylamino)phenyl]-, sodium salt (SCI)

(CA INDEX NAME)



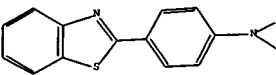
● Na

isolated ring systems:  
containing 1 : 10 :

Connectivity :  
18:5 M minimum C chain  
Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS 19:CLASS

L22 STRUCTURE UPLOADED

=> d  
L22 HAS NO ANSWERS  
L22 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 122 sss sam  
SAMPLE SEARCH INITIATED 14:59:51 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 784 TO 1736  
PROJECTED ANSWERS: 0 TO 0

L23 0 SEA SSS SAM L22

=> e 122 sss full  
FULL SEARCH INITIATED 14:59:55 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1240 TO ITERATE

100.0% PROCESSED 1240 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L24 0 SEA SSS FUL L22

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Uploading C:\Program Files\Stnexp\Queries\10.511852\clm16d.str

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COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 404.88 1195.54  
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL  
ENTRY SESSION  
CA SUBSCRIBER PRICE -49.92 -84.24

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STRUCTURE FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2  
DICTIONARY FILE UPDATES: 28 MAY 2007 HIGHEST RN 935999-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

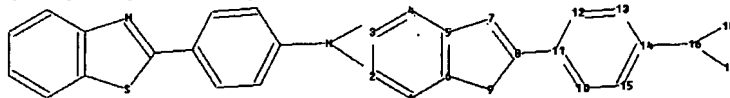
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

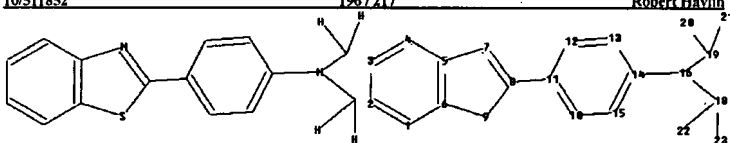
REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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16 18 19  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15  
chain bonds :  
8-11 14-16 16-18  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14  
14-15  
exact/norm bonds :  
5-7 7-8 14-16 16-18 16-19  
exact bonds :  
6-9 8-9 8-11  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

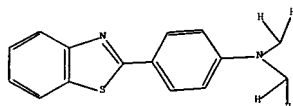


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8-11 14-16 16-18 16-19 18-22 18-23 19-20 19-21  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14  
14-15  
exact/norm bonds :  
5-7 7-8 14-16 16-18 16-19  
exact bonds :  
6-9 8-9 8-11 18-22 18-23 19-20 19-21  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15  
isolated ring systems :  
containing 1 : 10 :

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS  
23:CLASS

L25 STRUCTURE UPLOADED

=> d  
L25 HAS NO ANSWERS  
L25 STR



Structure attributes must be viewed using STN Express query preparation.



>> # 125 \*\*\* sam  
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 SAMPLE SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS 17 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 784 TO 1736  
 PROJECTED ANSWERS: 93 TO 587

L26 17 SEA SSS SAM L25

>> # 125 \*\*\* full  
 FULL SEARCH INITIATED 15:03:09 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 1240 TO ITERATE

100.0% PROCESSED 1240 ITERATIONS 323 ANSWERS  
 SEARCH TIME: 00.00.01

L27 323 SEA SSS FUL L25

>> d hist

(FILE 'HOME' ENTERED AT 14:20:05 ON 29 MAY 2007)

FILE 'USPATFULL, USPAT2' ENTERED AT 14:27:25 ON 29 MAY 2007

L1 0 S 4992204/PN  
 L2 0 S 4992204/PA  
 L3 1 S US4992204/PN

FILE 'REGISTRY' ENTERED AT 14:28:06 ON 29 MAY 2007

FILE 'USPATFULL' ENTERED AT 14:28:12 ON 29 MAY 2007  
 L4 TRA L3 1- RN : 74 TERMS

FILE 'REGISTRY' ENTERED AT 14:28:13 ON 29 MAY 2007

L5 74 SEA L4  
 L6 STRUCTURE UPLOADED  
 L7 4 S L6 SSS SAM  
 L8 127 S L6 SSS FULL

FILE 'HCAPLUS' ENTERED AT 14:31:44 ON 29 MAY 2007  
 L9 24 S L6

FILE 'REGISTRY' ENTERED AT 14:32:19 ON 29 MAY 2007

L10 STRUCTURE UPLOADED  
 L11 23 S L10 SSS SAM  
 L12 437 S L10 SSS FULL  
 L13 432 S L13 NOT L6

FILE 'HCAPLUS' ENTERED AT 14:38:26 ON 29 MAY 2007

L14 568 S L13  
 L15 388 S L14 AND PY <2002

FILE 'REGISTRY' ENTERED AT 14:41:13 ON 29 MAY 2007

L16 STRUCTURE UPLOADED  
 L17 12 S L16 SSS SAM  
 L18 226 S L16 SSS FULL  
 L19 206 S L13 NOT L18

FILE 'HCAPLUS' ENTERED AT 14:41:53 ON 29 MAY 2007

L20 75 S L19  
 L21 64 S L20 NOT PY > 2003

FILE 'REGISTRY' ENTERED AT 14:57:24 ON 29 MAY 2007

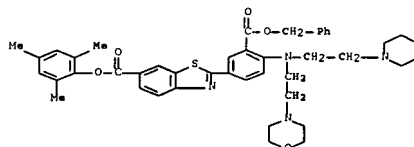
L22 STRUCTURE UPLOADED  
 L23 0 S L22 SSS SAM  
 L24 0 S L22 SSS FULL  
 L25 STRUCTURE UPLOADED  
 L26 17 S L25 SSS SAM  
 L27 323 S L25 SSS FULL

>> # 127 not 118

L28 97 L27 NOT L18

>> d scan

L28 97 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 6-Benzothiazolecarboxylic acid, 2-[4-[[bis(2-(4-morpholinyl)ethyl)amino]-3-benzothiazolyl]phenyl]imino]bis[ethanol] (2:1), block (9CI)  
 MF C43 H48 N4 O6 S

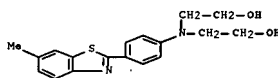


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L28 97 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Oxirane, methyl-, polymer with oxirane, ether with 2,2'-[[4-(6-methyl-2-benzothiazolyl)phenyl]imino]bis[ethanol] (2:1), block (9CI)  
 MF C18 H20 N2 O2 S . 2 (C3 H6 O . C2 H4 O) X

CM 1



CM 2

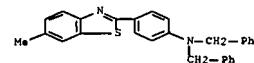
CM 3



CM 4



L28 97 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Benzothiazole, 2-[p-(diethylamino)phenyl]-6-methyl- (7CI, 8CI)  
 MF C28 H24 N2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

>> file hcaplus

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 FILE LAST UPDATED: 28 May 2007 (20070528/SD)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

>> # 128

L29 65 L28

>> # 129 not 121

L30 6 L29 NOT L21

>> d ibib abs hitstr tot

L30 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:623784 HCAPLUS Full-text

DOCUMENT NUMBER: 145:396965

TITLE: Femtosecond dynamics on 2-(2'-hydroxy-4'-diethylaminophenyl)benzothiazole: solvent polarity in the excited-state proton transfer

AUTHOR(S): Cheng, Yi-Ming; Pu, Shih-Chieh; Hsu, Chia-Jung; Lai, Chin-Hung; Chou, Pi-Tai

CORPORATE SOURCE: Department of Chemistry National Taiwan University, Taipei, Taiwan

SOURCE: ChemPhysChem (2006), 7(6), 1372-1381

CODEN: CPCHFT; ISSN: 1439-4235

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:396965

AB Detailed insights into the excited-state enol(N\*)-keto(T\*) intramol. proton transfer (ESIPT) reaction in 2-(2'-hydroxy-4'-diethylaminophenyl)benzothiazole (HABT) have been investigated via steady-state and femtosecond fluorescence uponconversion approaches. In cyclohexane, in contrast to the ultrafast rate of ESIPT for the parent 2-(2'-hydroxyphenyl)benzothiazole (> 2.9 x 0.3 + 1013 s-1), HABT undergoes a relatively slow rate (= 5.4 x 0.5 + 1011 s-1) of ESIPT. In polar aprotic solvents competitive rate of proton transfer and rate of solvent relaxation were resolved in the early dynamics. After reaching the solvation equilibrium in the normal excited state (Neq\*), ESIPT takes place with an appreciable barrier. The results also show Neq\*(enol) <=> Teq\*(keto) equilibrium, which shifts toward Neq\* as the solvent polarity increases. Temperature-dependent relaxation dynamics further resolved a solvent-induced barrier of 2.12 kcal mol-1 for the forward reaction in CHCl3. The observed spectroscopy and dynamics are rationalized by a significant difference in dipole moment between Neq\* and Teq\*, while the dipolar vector for the enol form in the ground state (N) is in between that of Neq\* and Teq\*. Upon N-N\* Franck-Condon excitation, ESIPT is energetically favorable, and its rate is competitive with the solvation relaxation process. Upon reaching equilibrium configurations Neq\* and Teq\*, forward and/or backward ESIPT takes place with an appreciable solvent polarity induced barrier due to differences in polarization equilibrium between Neq\* and Teq\*.

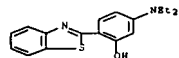
IT 55469-32-2P 149977-31-1P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

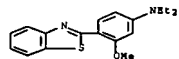
(excited-state proton transfer dynamics of 2-(2'-hydroxy-4'-diethylaminophenyl)benzothiazole)

RN 55469-32-2 HCAPLUS

CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



RN 149977-31-1 HCAPLUS  
CN Benzenamine, 4-(2-benzothiazolyl)-N,N-diethyl-3-methoxy- (9CI) (CA INDEX NAME)



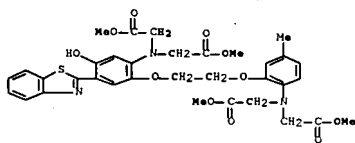
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:58103 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 142:130341  
TITLE: Metal-binding molecules and metal complexes and methods for detection and isolation of phosphorylated molecules  
INVENTOR(S): Agnew, Brian; Gee, Kyle R.; Martin, Vladimir V.  
PATENT ASSIGNER(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 96 pp., Cont.-in-part of U.S. Ser. No. 703,816.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005014197	A1	20050120	US 2004-821522	20040409
US 2004038306	A1	20040226	US 2003-428192	20030502
US 7102005	B2	20060905		
CA 2483868	A1	20040521	CA 2003-2483868	20030502
AU 2003299466	A1	20040607	AU 2003-299466	20030502
EP 1546118	A2	20050629	EP 2003-799756	20030502
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005539243	T	20051222	JP 2004-549877	20030502
US 2004171034	A1	20040902	US 2003-703816	20031107
IN 2004KN01676	A	20061110	IN 2004-KN1676	20041108
PRIORITY APPL. INFO.:				
			US 2002-377733P	P 20020503
			US 2002-393059P	P 20020628
			US 2002-407255P	P 20020830
			US 2003-440252P	P 20030114
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			WO 2003-US13765	W 20030502

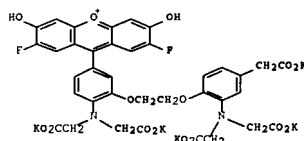
OTHER SOURCE(S): MARPAT 142:130341

IT 663625-90-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(Reactant or reagent)  
(metal-binding mole. and metal complexes and methods for detection and isolation of phosphorylated mole.)  
RN 663625-90-9 HCAPLUS  
CN Glycine, N-[2-[2-[5-(2-benzothiazolyl)-2-[bis(2-methoxy-2-oxoethyl)amino]-4-hydroxyphenoxy]ethoxy]-4-methylphenyl]-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)



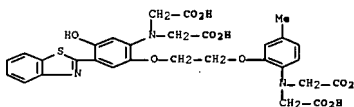
L30 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:722822 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 141:239312  
TITLE: Compositions and methods for detection and isolation of phosphorylated molecules  
INVENTOR(S): Agnew, Brian; Beechen, Joseph; Gee, Kyle; Haugland, Richard; Steinberg, Thomas; Patton, Wayne  
PATENT ASSIGNER(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 89 pp., Cont.-in-part of U.S. Ser. No. 428,192.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004171034	A1	20040902	US 2003-703816	20031107
US 2004038306	A1	20040226	US 2003-428192	20030502
US 7102005	B2	20060905		
CA 2483868	A1	20040521	CA 2003-2483868	20030502
AU 2003299466	A1	20040607	AU 2003-299466	20030502
EP 1546118	A2	20050629	EP 2003-799756	20030502
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005539243	T	20051222	JP 2004-549877	20030502
US 2005014197	A1	20050120	US 2004-821522	20040409
WO 2005047901	A2	20050526	WO 2004-US36968	20041105
WO 2005047901	A3	20050728		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MY, NA, NI,				



AB The present invention relates to phosphate-binding compds. that find use in binding, detecting and isolating phosphorylated target mole., including the subsequent identification of target mole. that interact with phosphorylated target mole. or mole. capable of being phosphorylated. The phosphate-binding compds. comprise a metal-chelating moiety such as BAPTA, DTPA, IDA, and phenanthroline. This metal-chelating moiety is desirably attached to a label, e.g., a dye or a hapten and/or a reactive group. Preferred dyes are benzofurans, quinoxalines, xanthenes, indoles, benzoxoles, and borapolyazaindenees. A binding solution is provided that comprises a phosphate-binding compound, an acid and a metal ion wherein the metal ion simultaneously interacts with an exposed phosphate group on a target mol. and the metal chelating moiety of the phosphate-binding compound forming a bridge between the phosphate-binding compound and a phosphorylated target mol. resulting in a ternary complex. The binding solution of the present invention finds use in binding and detecting immobilized and solubilized phosphorylated target mole., isolation of phosphorylated target mole. from a complex mixture and aiding in proteomic anal. wherein kinase and phosphatase substrates and enzymes can be identified. Thus, a compound comprising dihydroxydifluoroxanthene attached to BAPTA and dextran (I) was prepared. I might be used, after addition of GdCl3 to form complexes, as an affinity matrix to isolate phosphopeptides. The phosphopeptides might then be identified by mass spectrometry.

IT 663625-32-9P  
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(metal-binding mole. and metal complexes and methods for detection and isolation of phosphorylated mole.)  
RN 663625-32-9 HCAPLUS  
CN Glycine, N-[2-[2-[5-(2-benzothiazolyl)-2-[bis(carboxymethyl)amino]-4-hydroxyphenoxy]ethoxy]-4-methylphenyl]-N-(carboxymethyl)-, tetrapotassium salt (9CI) (CA INDEX NAME)

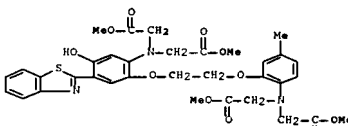


● 4 K

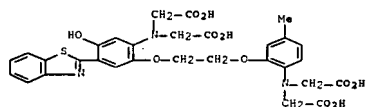
NO, NZ, OM, PO, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
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IN 2004KN01676 A 20061110 IN 2004-KN1676 20041108  
US 2007054304 A1 20070308 US 2006-552275 20061024  
US 2003-377733P P 20020503  
PRIORITY APPL. INFO.:

US 2002-393059P P 20020628  
US 2002-407255P P 20020830  
US 2003-440252P P 20030114  
US 2003-428192 A2 20030502  
WO 2003-US13765 W 20030502  
US 2003-703816 A2 20031107  
AB The present invention relates to phosphate-binding compds. that find use in binding, detecting and isolating phosphorylated target mole., including the subsequent identification of target mole. that interact with phosphorylated target mole. or mole. capable of being phosphorylated. A binding solution is provided that comprises a phosphate-binding compound, an acid and a metal ion wherein the metal ion simultaneously interacts with an exposed phosphate group on a target mol. and the metal chelating moiety of the phosphate-binding compound forming a bridge between the phosphate-binding compound and a phosphorylated target mol. resulting in a ternary complex. The binding solution of the present invention finds use in binding and detecting immobilized and solubilized phosphorylated target mole., isolation of phosphorylated target mole. from a complex mixture and aiding in proteomic anal. wherein kinase and phosphatase substrates and enzymes can be identified.

IT 663625-90-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(compns. and methods for detection and isolation of phosphorylated mole.)  
RN 663625-90-9 HCAPLUS  
CN Glycine, N-[2-[2-[5-(2-benzothiazolyl)-2-[bis(2-methoxy-2-oxoethyl)amino]-4-hydroxyphenoxy]ethoxy]-4-methylphenyl]-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)



IT 663625-32-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(compns. and methods for detection and isolation of phosphorylated mole.)  
RN 663625-32-9 HCAPLUS  
CN Glycine, N-[2-[2-[5-(2-benzothiazolyl)-2-[bis(carboxymethyl)amino]-4-hydroxyphenoxy]ethoxy]-4-methylphenyl]-N-(carboxymethyl)-, tetrapotassium salt (9CI) (CA INDEX NAME)

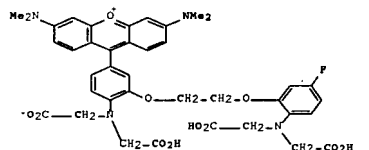


4 K

L30 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:162337 HCAPLUS Full-text  
 DOCUMENT NUMBER: 140:213577  
 TITLE: Compositions and methods for detection and isolation of phosphorylated molecules  
 INVENTOR(S): Agnew, Brian; Beechem, Joseph; Oee, Kyle; Haugland, Richard; Liu, Jixiang; Martin, Vladimir; Patton, Wayne; Steinberg, Thomas  
 PATENT ASSIGNEE(S): Molecular Probes, Inc., USA  
 SOURCE: U.S. Pat. Appl. Publ., 83 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

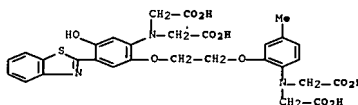
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US 2004038306	A1	20040226	US 2003-428192	20030502
US 7102005	B2	20060905		
CA 2483868	A1	20040521	CA 2003-2483868	20030502
MO 2004042347	A2	20040521	MO 2003-US13765	20030502
MO 2004042347	A3	20050414		
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RM: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TO				
AU 2003299466	A1	20040607	AU 2003-299466	20030502
EP 1546118	A2	20050629	EP 2003-799756	20030502
R:				
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CN 1665790	A	20050907	CN 2003-815684	20030502
JP 2005539243	T	20051222	JP 2004-549877	20030502
US 2004171034	A1	20040902	US 2003-703816	20031107
US 2005014197	A1	20050120	US 2004-821522	20040409
IN 2004KN01676	A	20061110	IN 2004-KN1676	20041108
US 2007054304	A1	20070308	US 2006-552275	20061024
PRIORITY APPLN. INFO.:				
			US 2002-377733P	P 20020503
			US 2002-393059P	P 20020628
			US 2002-407255P	P 20020830
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			US 2003-428192	A2 20030502

OTHER SOURCE(S): MARPAT 140:213577  
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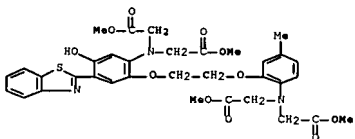
AB The present invention relates to phosphate-binding compounds that find use in binding, detecting and isolating phosphorylated target molecules, including the subsequent identification of target molecules that interact with phosphorylated target molecules, or molecules capable of being phosphorylated. A binding solution is provided that comprises a phosphate-binding compound, an acid and a metal ion wherein the metal ion simultaneously interacts with an exposed phosphate group on a target molecule and the metal chelating moiety of the phosphate-binding compound forming a bridge between the phosphate-binding compound and a phosphorylated target molecule, resulting in a ternary complex. The binding solution of the present invention finds use in binding and detecting immobilized and solubilized phosphorylated target molecules, isolation of phosphorylated target molecules from a complex mixture and aiding in proteomic analysis wherein kinase and phosphatase substrates and enzymes can be identified. A human MRC-5 lung fibroblast cell lysate protein mixture was separated by two-dimensional gel electrophoresis. The gel was fixed and then phosphoproteins were stained with a solution containing 50 mM NaOAc, pH 4.0, 250 mM NaCl, 20% volume/volume 1,2-propanediol, 1 μM rhodamine-BAPTA chelating compound I, and 1 μM gallium chloride.

IT 663625-32-9P  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (metal ions, acids, and chelating phosphate-binding agents for detection and isolation of phosphorylated molecules.)  
 RN 663625-32-9 HCAPLUS  
 CN Glycine, N-[2-(2-[5-(2-benzothiazolyl)-2-[bis(carboxymethylamino)-4-hydroxyphenoxy]ethoxy]-4-methylphenyl)-N-(carboxymethyl)-, tetrapotassium salt (9CI) (CA INDEX NAME)



4 K

IT 663625-90-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (metal ions, acids, and chelating phosphate-binding agents for detection and isolation of phosphorylated molecules.)  
 RN 663625-90-9 HCAPLUS  
 CN Glycine, N-[2-(2-[5-(2-benzothiazolyl)-2-[bis(2-methoxy-2-oxoethylamino)-4-hydroxyphenoxy]ethoxy]-4-methylphenyl)-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)



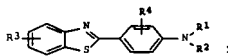
REFERENCE COUNT: 208 THERE ARE 208 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RS FORMAT

L30 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2003:836808 HCAPLUS Full-text  
 DOCUMENT NUMBER: 139:327931  
 TITLE: Aminophenyl-benzothiazole compounds as UV filters in cosmetics  
 INVENTOR(S): Wagner, Barbara; Ehli, Thomas; Mongiat, Sebastian; Richin, Kai  
 PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Swiss.  
 SOURCE: PCT Int. Appl., 48 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
MO 2003086341	A2	20031023	MO 2003-EP3870	20030414
MO 2003086341	A3	20040401		
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RM: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KO, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TO				
AU 2003229665	A1	20031027	AU 2003-229665	20030414
EP 1494641	A2	20050112	EP 2003-722472	20030414

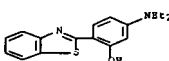
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 BR 2003009308 A 20050215 BR 2003-9308 20030414  
 CN 1646507 A 20050727 CN 2003-806554 20030414  
 US 2005175554 A1 20050811 US 2003-511852 20030414  
 JP 200529869 T 20051006 JP 2003-583365 20030414  
 IN 2004CN02585 A 20070302 IN 2004-CN2585 20041117  
 PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 139:327931  
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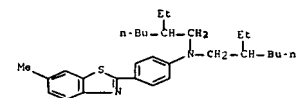


AB The preparation and use, as a UV filter, of a compound of formula I (R1, R2 = H, unsubstituted or halo-, amino-, mono- or di-C1-5-alkylamino-, cyano- or C1-5-alkoxy-substituted C1-22-alkyl, C5-10-cycloalkyl, carboxy-C1-22-alkyl, carboxy-C6-10-aryl, C6-10-aryl, C6-10-aryl-C1-5-alkyl; carbamoyl; sulfamoyl; R1, R2, N forming 5- to 7-membered heterocyclic radical; R3 = H, C1-22-alkyl; R4 = H, OH, C1-22-alkyl, C1-22-alkoxy) is described. The compounds of formula I in micronized form are suitable as UV absorbers in cosmetic preparations and for protecting hair and skin from UV radiation.

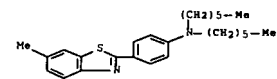
IT 55489-32-2P 614717-93-OP 614717-94-1P 614717-95-2P 614717-96-3P 614717-97-4P 614717-98-5P 614717-99-6P  
 RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and cosmetic use of aminophenyl benzothiazole compounds as UV filters)  
 RN 55489-32-2 HCAPLUS  
 CN Phenol, 2-(2-benzothiazolyl)-5-(diethylamino)- (9CI) (CA INDEX NAME)



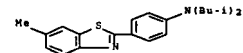
RN 614717-93-0 HCAPLUS  
 CN Benzeneimine, N,N-bis(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



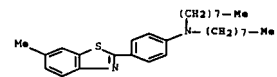
RN 614717-94-1 HCAPLUS  
CN Benzenamine, N,N-dihexyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



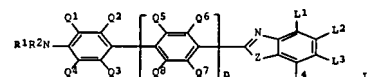
RN 614717-95-2 HCAPLUS  
CN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-N,N-bis(2-methylpropyl)- (9CI) (CA INDEX NAME)



RN 614717-96-3 HCAPLUS  
CN Benzenamine, 4-(6-methyl-2-benzothiazolyl)-N,N-diethyl- (9CI) (CA INDEX NAME)



RN 614717-97-4 HCAPLUS  
CN Benzenamine, N,N-didodecyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)

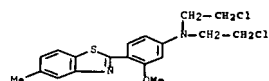


AB The media have a recording layer and a reflection layer on a substrate, in which the recording layer contain an aromatic derivative having I (L1-4 = H, halogen, cyano, alkyl, aralkyl, aryl, alkoxy, aralkyloxy, aryloxy, alkenyl, alkenyloxy, alkylthio, aralkylthio, arylthio, alkylamino, aralkylamino, arylamino, alkenylamino, acyl, alkoxy, carbonyl, aralkyloxy, carbonyl, aryloxy, carbonyl, alkenyloxy, carbonyl, alkylaminocarbonyl, heterocyclic, alkylsulfonyl, arylsulfonyl; Q1-8 = H, halogen, cyano, alkyl, aralkyl, aryl, alkoxy, aralkyloxy, aryloxy, alkenyl, alkenyloxy, alkylthio, aralkylthio, arylthio, alkylamino, aralkylamino, arylamino, alkenylamino, acyl, alkoxy, carbonyl, aralkyloxy, carbonyl, aryloxy, carbonyl, alkenyloxy, carbonyl, alkylaminocarbonyl, heterocyclic; R1, 2 = H, O, alkyl, aralkyl, alkenyl, aryl, alkoxy, carbonyl, aralkyloxy, carbonyl, aryloxy, carbonyl, alkenyloxy, carbonyl; R1 and R2 may bond to form a ring; Z = O, S; n = 0, 1). The media show high reflection and excellent durability. The media are useful for recording and reading information using blue-light-emitting laser.

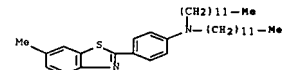
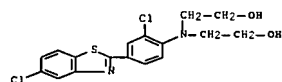
IT 272444-96-9 272444-97-0 272444-98-1  
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272445-08-6 272445-09-7 272445-10-0  
272445-11-1 272445-12-2 272445-13-3  
272445-14-4 272445-15-5 272445-16-6  
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RL: DEV (Device component use); MQA (Modifier or additive use); USES (rewritable optical recording media containing aromatic derivative)

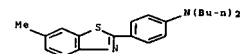
RN 272444-96-9 HCAPLUS  
CN Benzenamine, N,N-bis(2-chloroethyl)-3-methoxy-4-(5-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



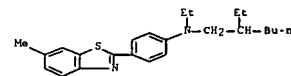
RN 272444-97-0 HCAPLUS  
CN Ethanol, 2,2'-[2-chloro-4-(5-chloro-2-benzothiazolyl)phenyl]imino]bis- (9CI) (CA INDEX NAME)



RN 614717-98-5 HCAPLUS  
CN Benzenamine, N,N-dibutyl-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 614717-99-6 HCAPLUS  
CN Benzenamine, N-ethyl-N-(2-ethylhexyl)-4-(6-methyl-2-benzothiazolyl)- (9CI) (CA INDEX NAME)

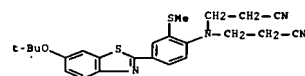


L30 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2000:362695 HCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 133:24759  
TITLE: Optical recording media containing aromatic derivative  
INVENTOR(S): Ogiso, Akira; Tsukahara, Hiroshi; Mishimoto, Taizo; Miesawa, Teiyo; Takuma, Keisuke  
PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan; Yamamoto Chemicals Inc.  
SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

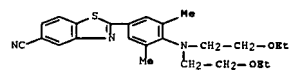
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PRIORITY APPLN. INFO.:  
OTHER SOURCE(S): MARPAT 133:24759  
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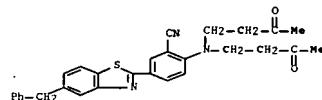
RN 272444-98-1 HCAPLUS  
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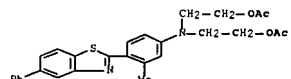
RN 272444-99-2 HCAPLUS  
CN 5-Benzothiazolecarbonitrile, 2-[4-[bis(2-ethoxyethyl)amino]-3,5-dimethylphenyl]- (9CI) (CA INDEX NAME)



RN 272445-00-8 HCAPLUS  
CN Benzonitrile, 2-[bis(3-oxobutyl)amino]-5-[5-(phenylmethyl)-2-benzothiazolyl]- (9CI) (CA INDEX NAME)

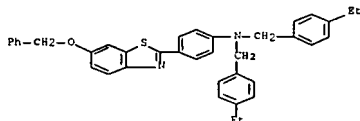


RN 272445-01-9 HCAPLUS  
CN Ethanol, 2,2'-[[3-methyl-4-(5-phenyl-2-benzothiazolyl)phenyl]imino]bis-, diacetate (ester) (9CI) (CA INDEX NAME)



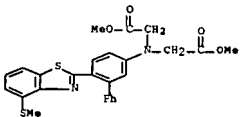
RN 272445-02-0 HCAPLUS  
CN Benzenemethanamine, 4-ethyl-N-[(4-ethylphenyl)methyl]-N-[4-(6-

(phenylmethoxy)-2-benzothiazolyl]phenyl]- (9CI) (CA INDEX NAME)



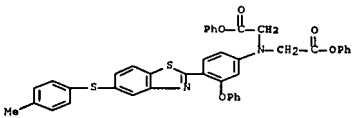
RN 272445-06-4 HCAPLUS

CN Glycine, N-(2-methoxy-2-oxoethyl)-N-[6-(4-(methylthio)-2-benzothiazolyl)[1,1'-biphenyl]-3-yl]-, methyl ester (9CI) (CA INDEX NAME)



RN 272445-07-5 HCAPLUS

CN Glycine, N-[4-[5-[(4-methylphenyl)thio]-2-benzothiazolyl]-3-phenoxyphenyl]-N-(2-oxo-2-phenoxyethyl)-, phenyl ester (9CI) (CA INDEX NAME)

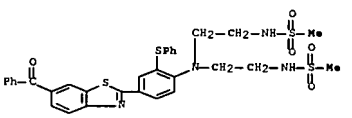


RN 272445-08-6 HCAPLUS

CN β-Alanine, N-[4-[6-(dibutylamino)-2-benzothiazolyl]-2-(phenylmethoxy)phenyl]-N-[3-oxo-3-(2-propenyloxy)propyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

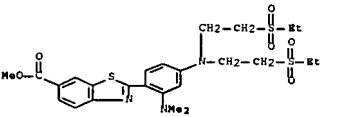


CN Methanesulfonamide, N,N'-[[[4-(6-benzoyl-2-benzothiazolyl)-2-(phenylthio)phenyl]imino]di-2,1-ethanediy]bis- (9CI) (CA INDEX NAME)



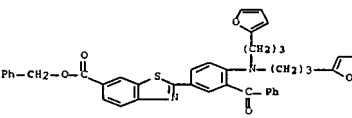
RN 272445-13-3 HCAPLUS

CN 6-Benzothiazolecarboxylic acid, 2-[4-[bis[2-(ethylsulfonyl)ethyl]amino]-2-(dimethylamino)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



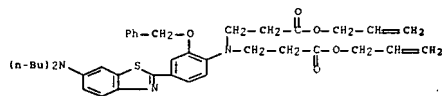
RN 272445-14-4 HCAPLUS

CN 6-Benzothiazolecarboxylic acid, 2-[3-benzoyl-4-[bis[3-(2-furyl)propyl]amino]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



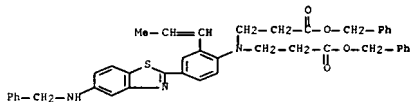
RN 272445-15-5 HCAPLUS

CN 6-Benzothiazolecarboxylic acid, 2-[4-[bis[2-(4-morpholinyl)ethyl]amino]-3-[(phenylmethoxy)carbonyl]phenyl]-, 2,4,6-trimethylphenyl ester (9CI) (CA INDEX NAME)



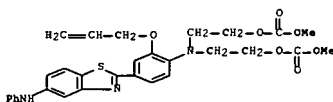
RN 272445-09-7 HCAPLUS

CN β-Alanine, N-[3-oxo-3-(phenylmethoxy)propyl]-N-[4-[5-(phenylmethyl)amino]-2-benzothiazolyl]-2-(1-propenyl)phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



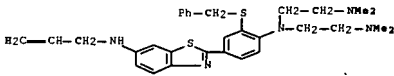
RN 272445-10-0 HCAPLUS

CN 2,4,10-Trioxa-7-azadecan-11-oic acid, 3-oxo-7-[4-[5-(phenylamino)-2-benzothiazolyl]-2-(2-propenyloxy)phenyl]-, methyl ester (9CI) (CA INDEX NAME)

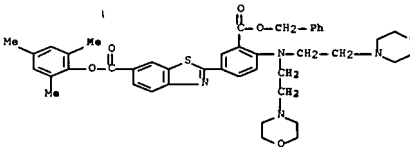


RN 272445-11-1 HCAPLUS

CN 1,2-Ethanediamine, N-[2-(dimethylamino)ethyl]-N',N'-dimethyl-N-[2-[(phenylmethyl)thio]-4-[6-(2-propenyloxy)-2-benzothiazolyl]phenyl]- (9CI) (CA INDEX NAME)

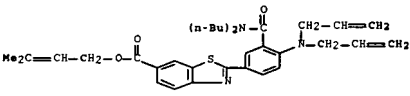


RN 272445-12-2 HCAPLUS



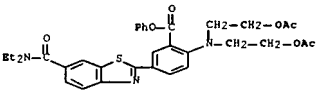
RN 272445-16-6 HCAPLUS

CN 6-Benzothiazolecarboxylic acid, 2-[3-[(dibutylamino)carbonyl]-4-(di-2-propenyloxy)phenyl]-, 3-methyl-2-butenyl ester (9CI) (CA INDEX NAME)



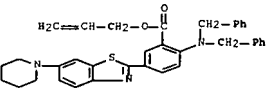
RN 272445-17-7 HCAPLUS

CN Benzoic acid, 2-[bis[2-(acetyloxy)ethyl]amino]-5-[6-[(diethylamino)carbonyl]-2-benzothiazolyl]-, phenyl ester (9CI) (CA INDEX NAME)



RN 272445-18-8 HCAPLUS

CN Benzoic acid, 2-[bis(phenylmethyl)amino]-5-[6-(1-piperidinyl)-2-benzothiazolyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)



Robert Havlin

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 15:05:17 ON 29 MAY 2007